

Figure 1

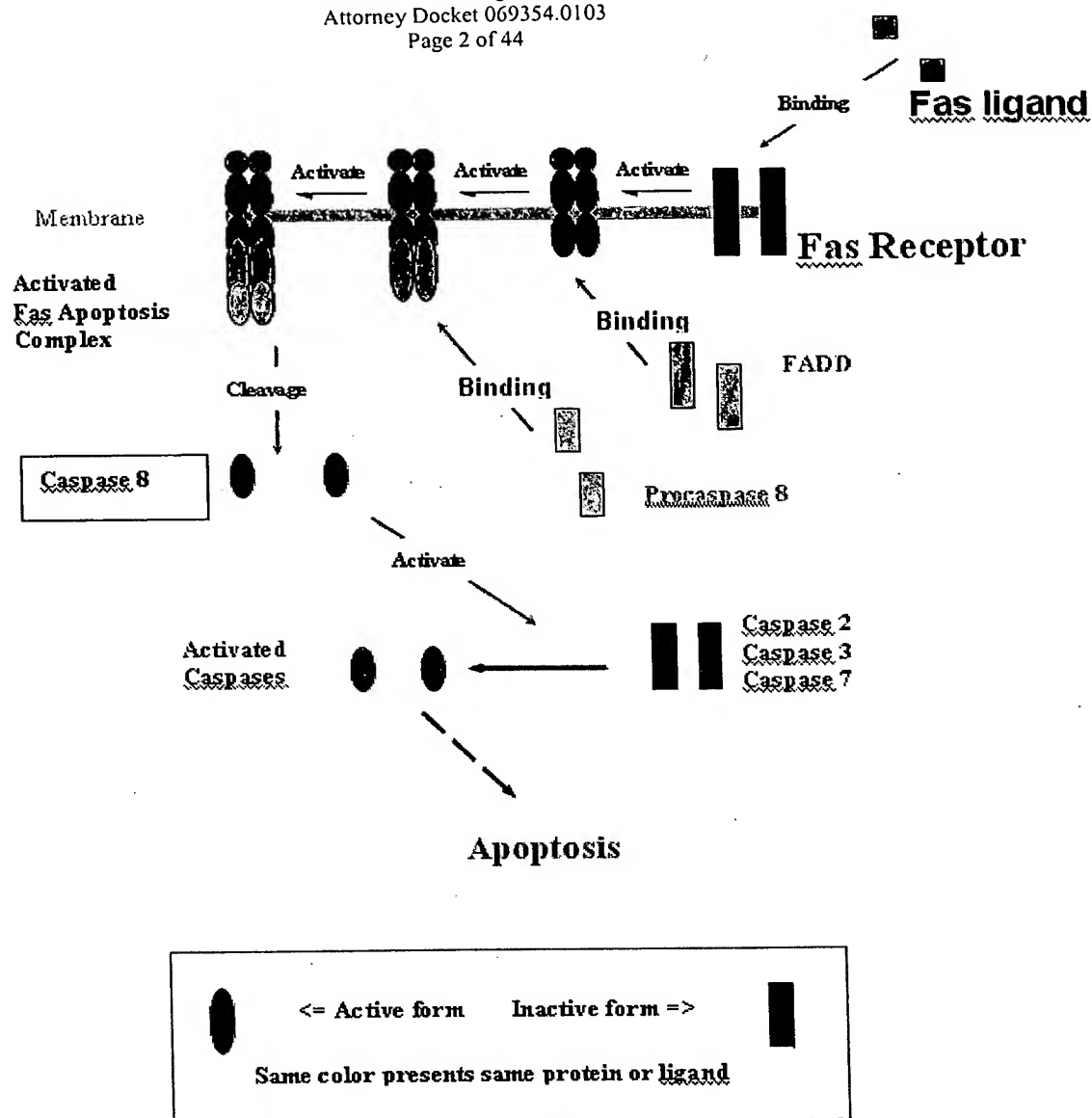


Figure 2



***Methods for Simulation of Biological and/or
Chemical Reaction Pathway, Biomolecules and
Nano-Molecular Systems***

Inventors: Yu Zong Chen et al.

Attorney Docket 069354.0103

Page 4 of 44

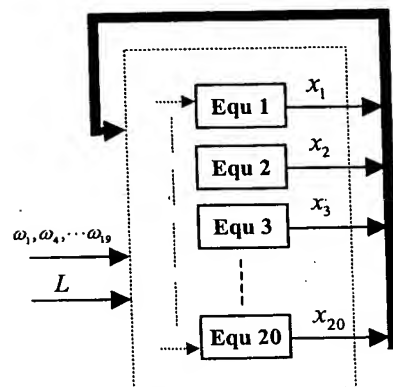


Figure 4

*Methods for Simulation of Biological and/or
Chemical Reaction Pathway, Biomolecules and
Nano-Molecular Systems*
Inventors: Yu Zong Chen et al.
Attorney Docket 069354.0103
Page 5 of 44

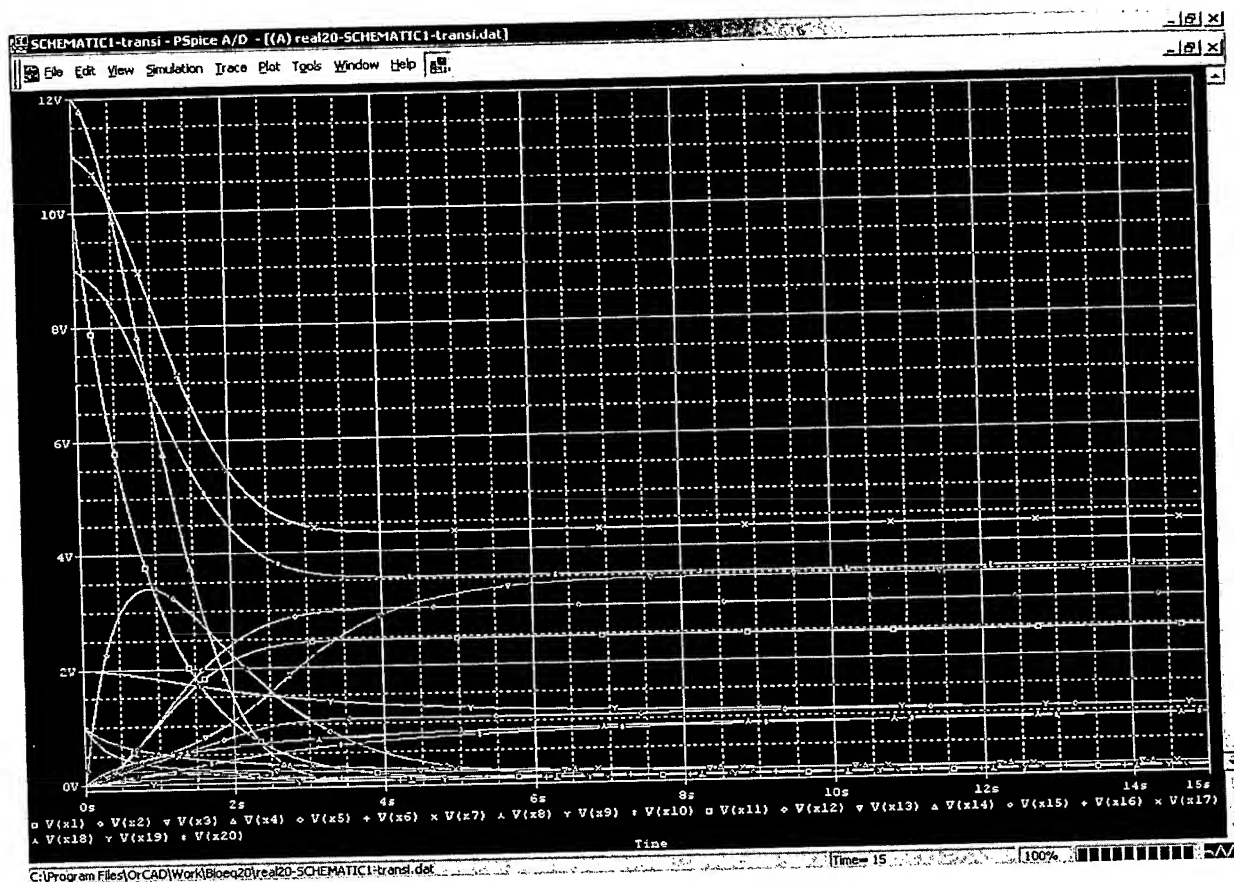


Figure 5

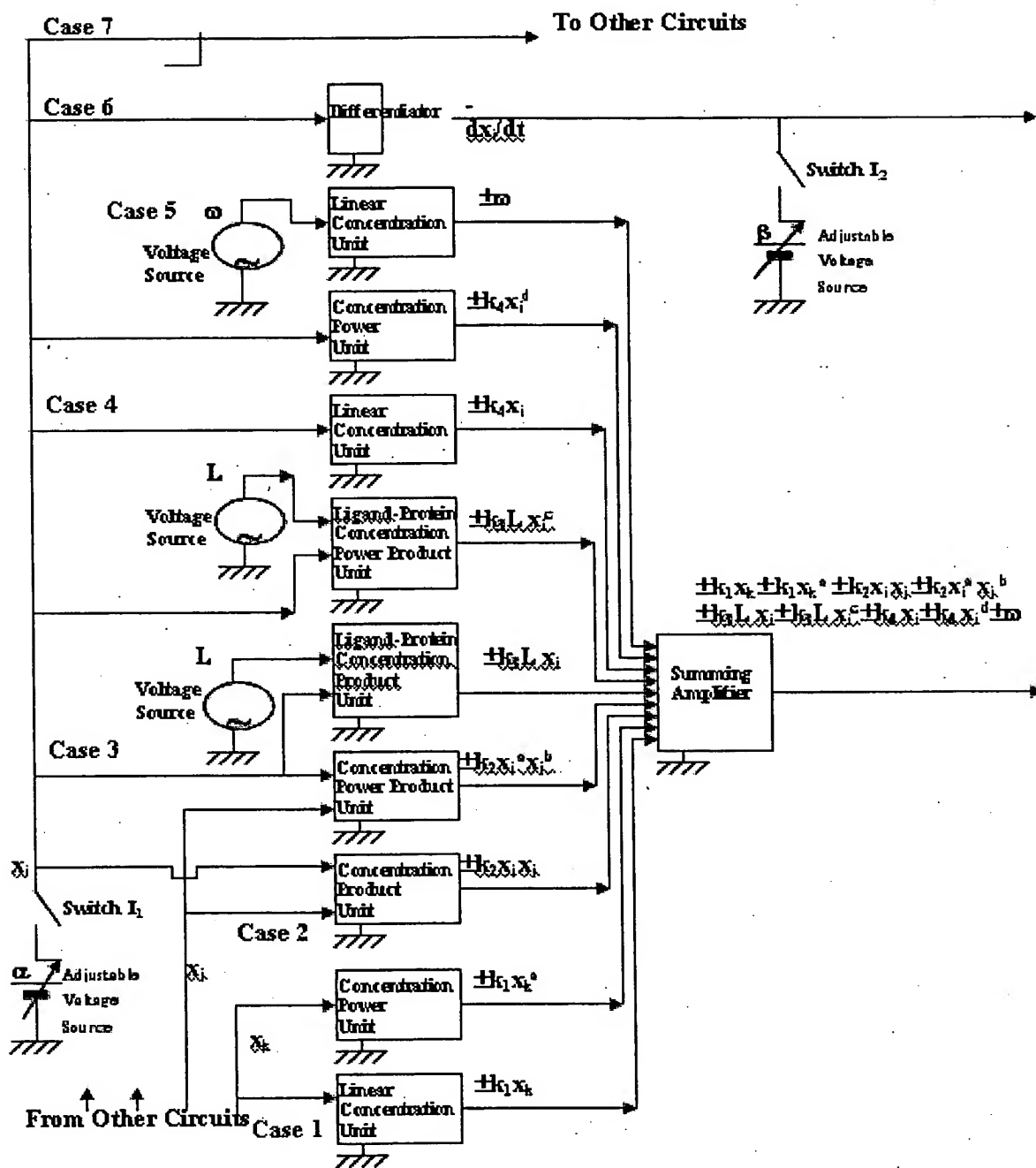


Figure 6

*Methods for Simulation of Biological and/or
Chemical Reaction Pathway, Biomolecules and
Nano-Molecular Systems*

Inventors: Yu Zong Chen et al.

Attorney Docket 069354.0103

Page 7 of 44

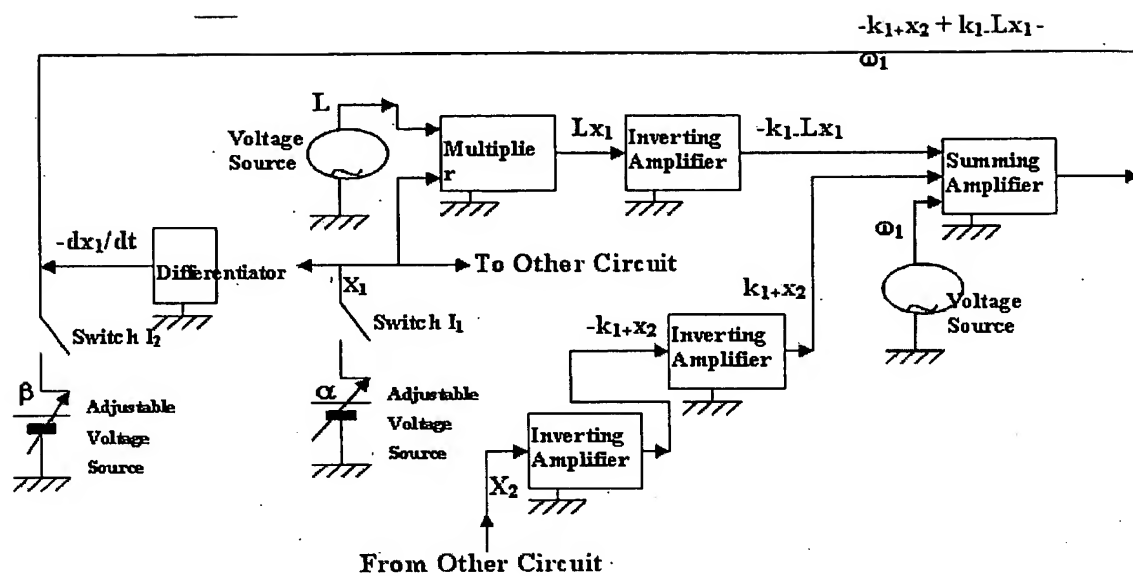


Figure 7

*Methods for Simulation of Biological and/or
Chemical Reaction Pathway, Biomolecules and
Nano-Molecular Systems*

Inventors: Yu Zong Chen et al.

Attorney Docket 069354.0103

Page 8 of 44

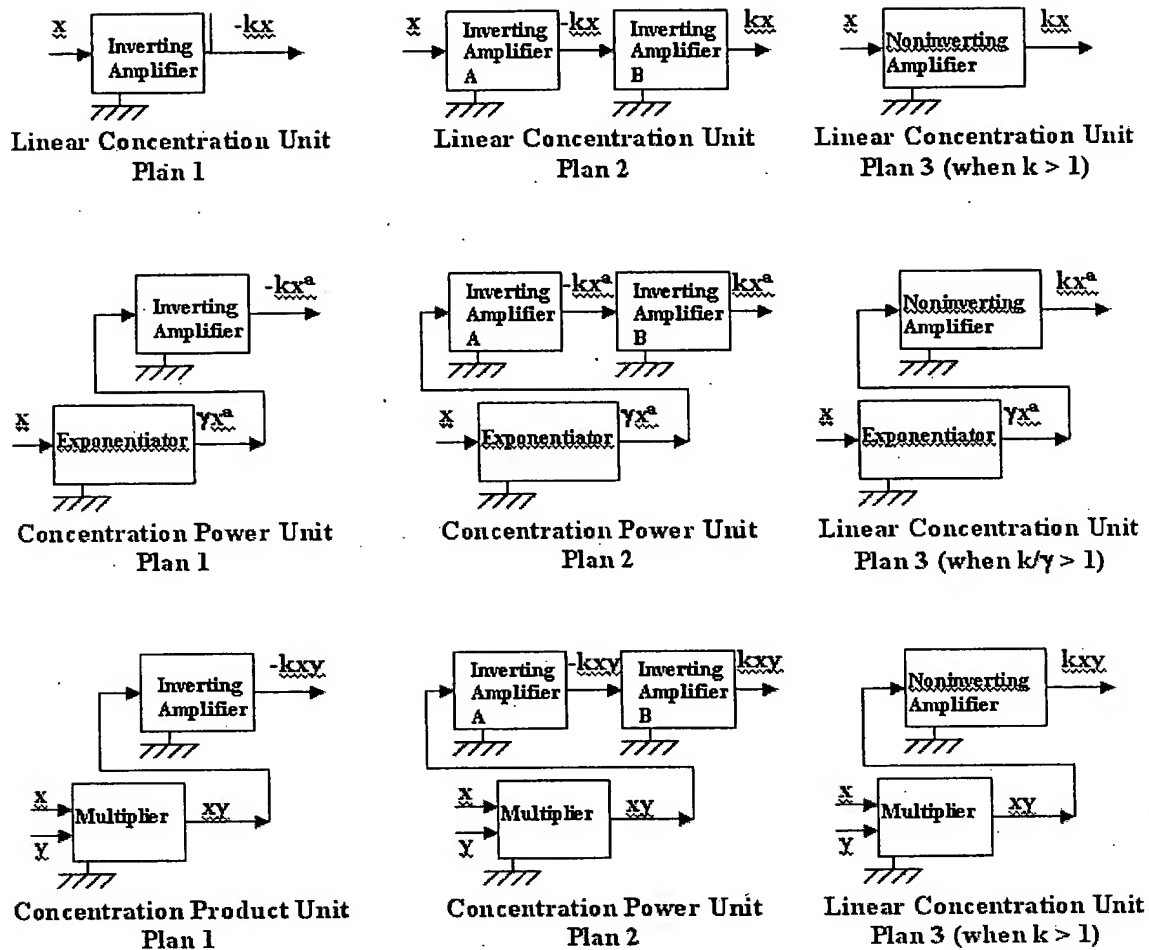


Figure 8

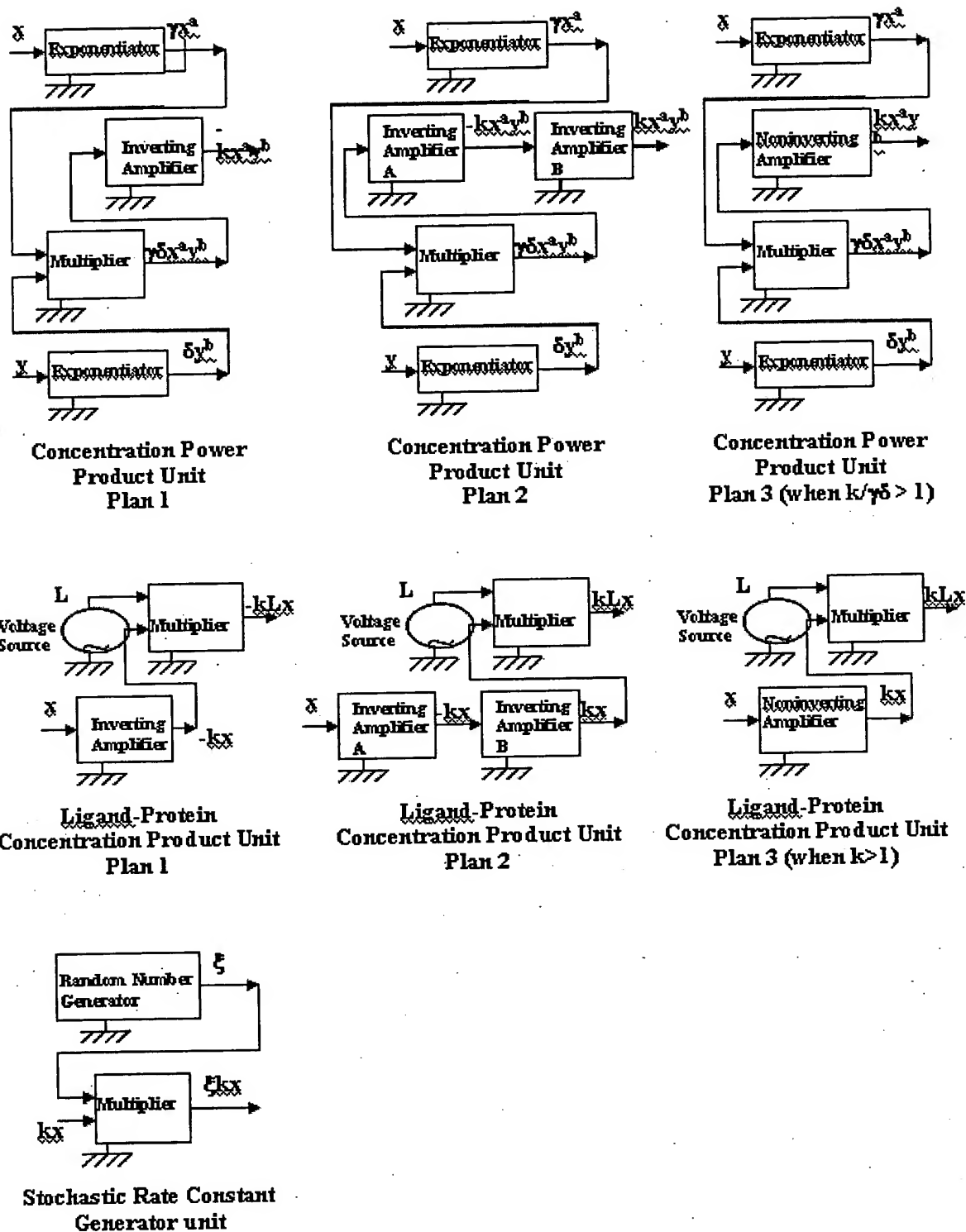
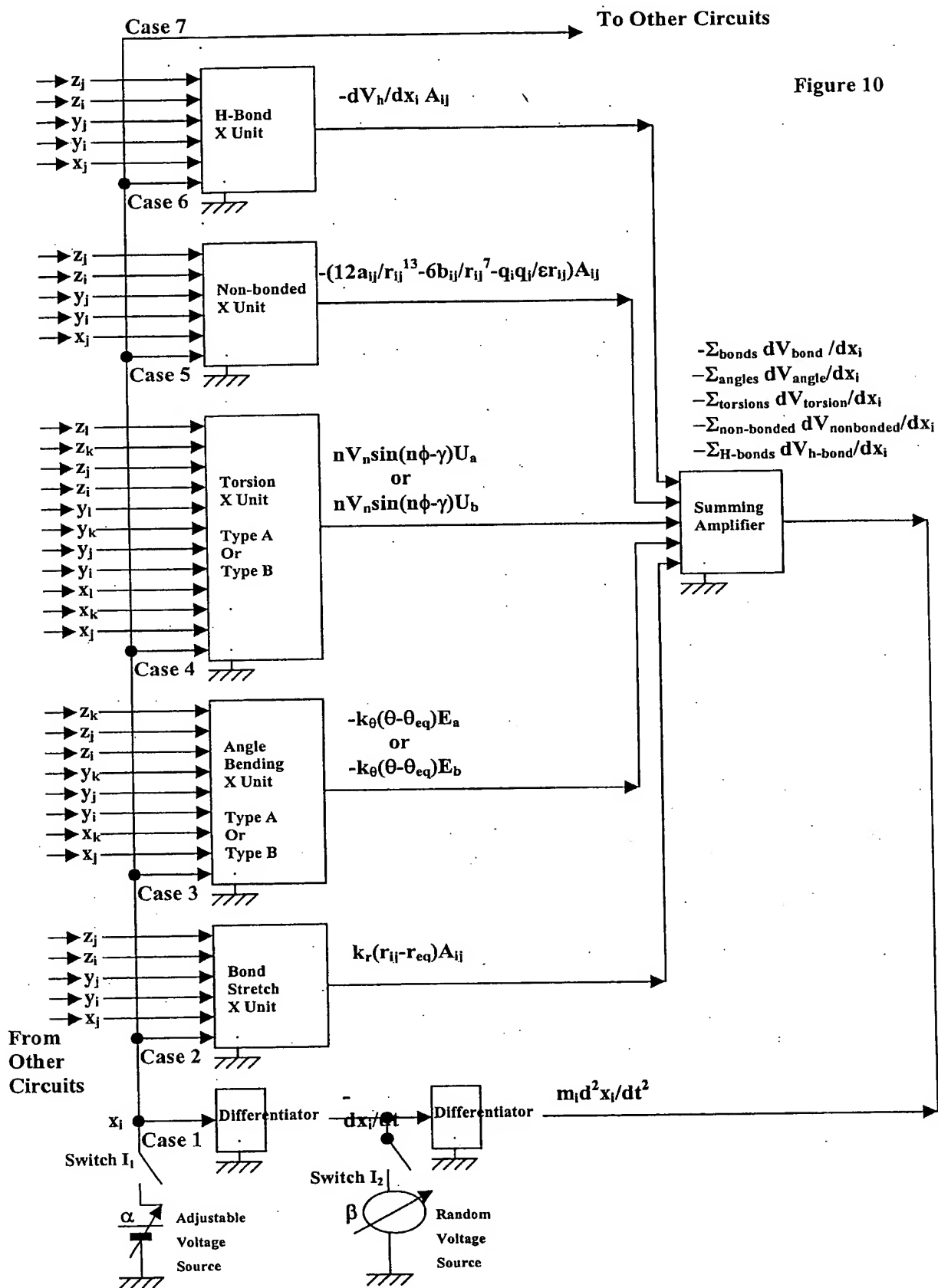
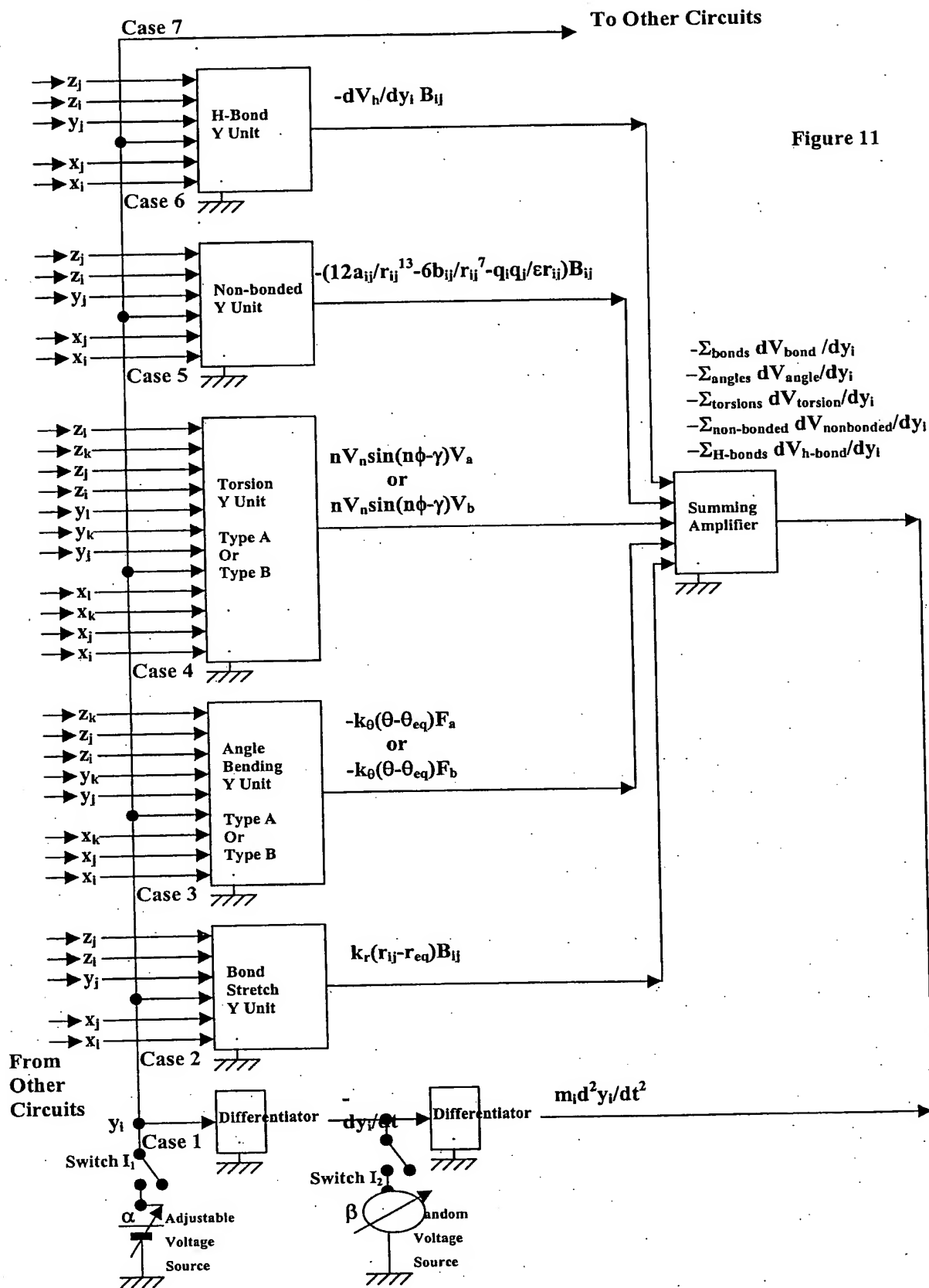
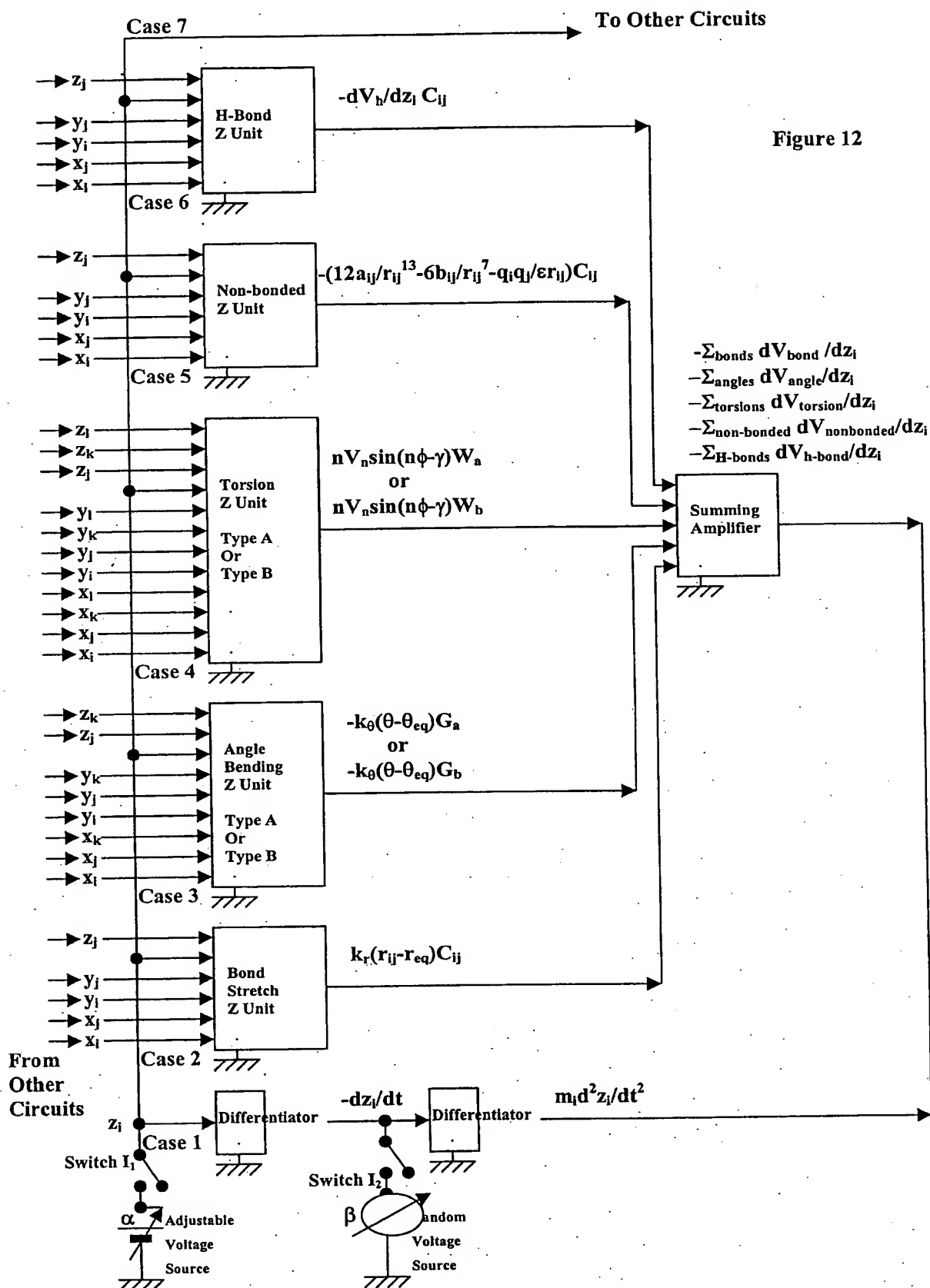


Figure 9







**Illustration of the Circuit Group
For an Amino Acid
(Bond Stretch Connections)**

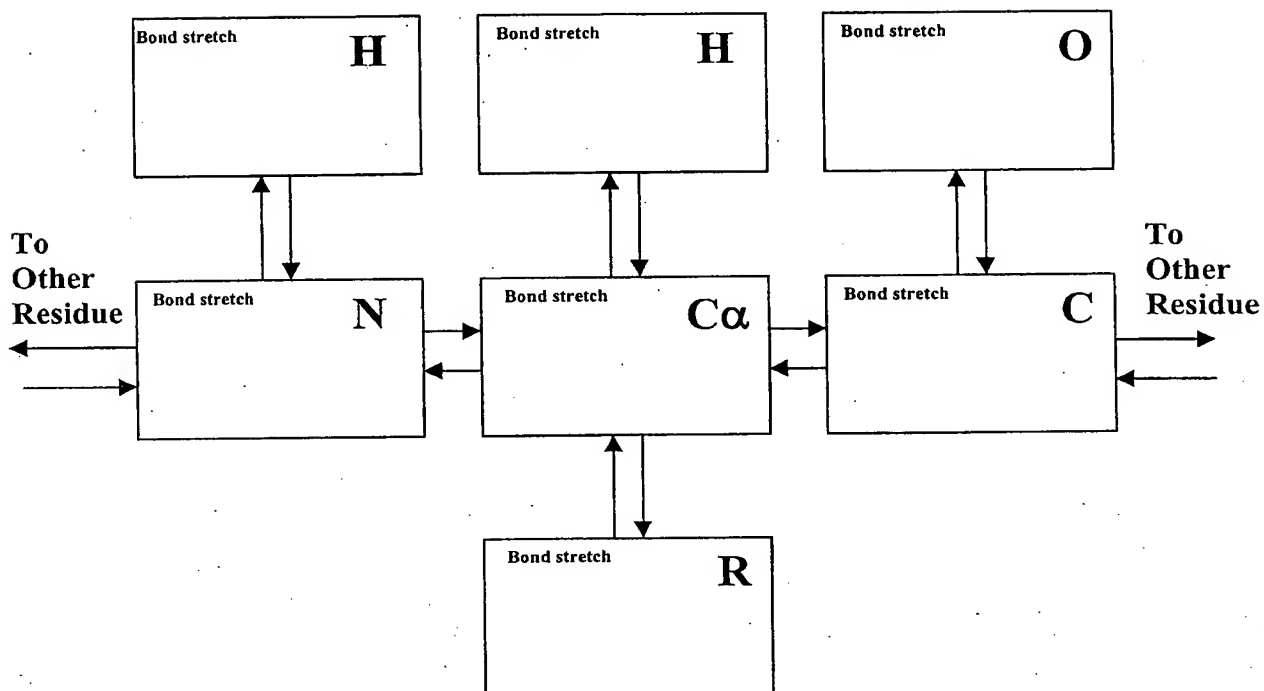


Figure 13

**Illustration of the Circuit Group
For an Amino Acid
(Angle Bending Connections)**

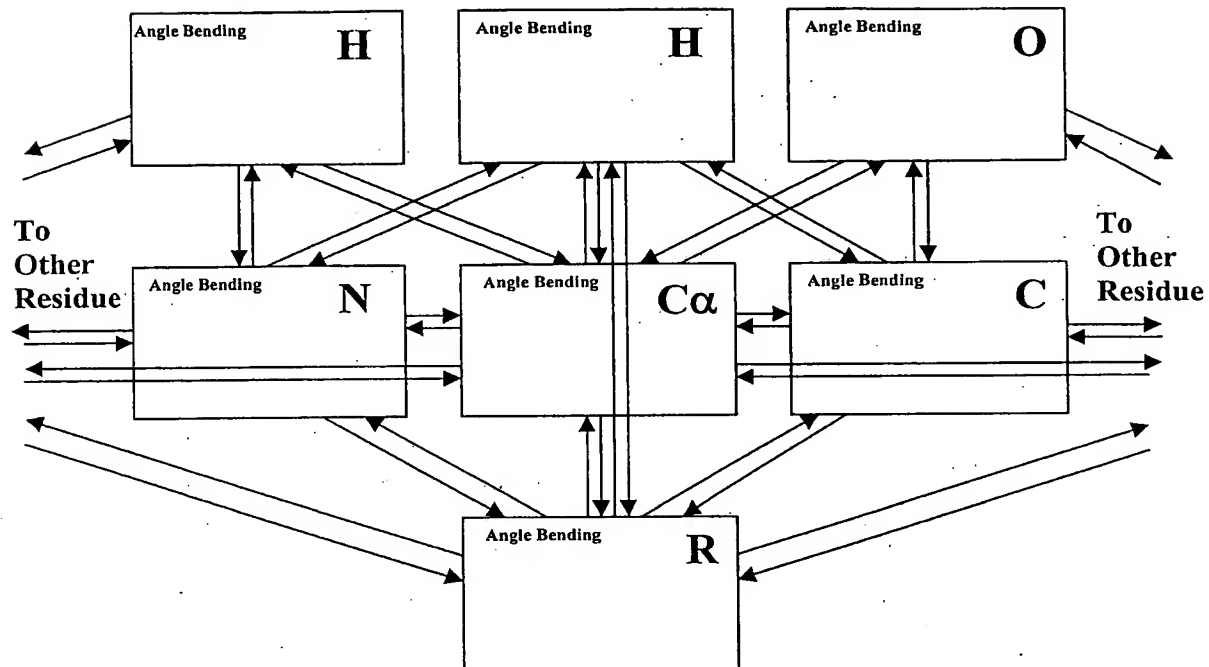


Figure 14

**Illustration of the Circuit Group
For an Amino Acid
(Torsion Connections)**

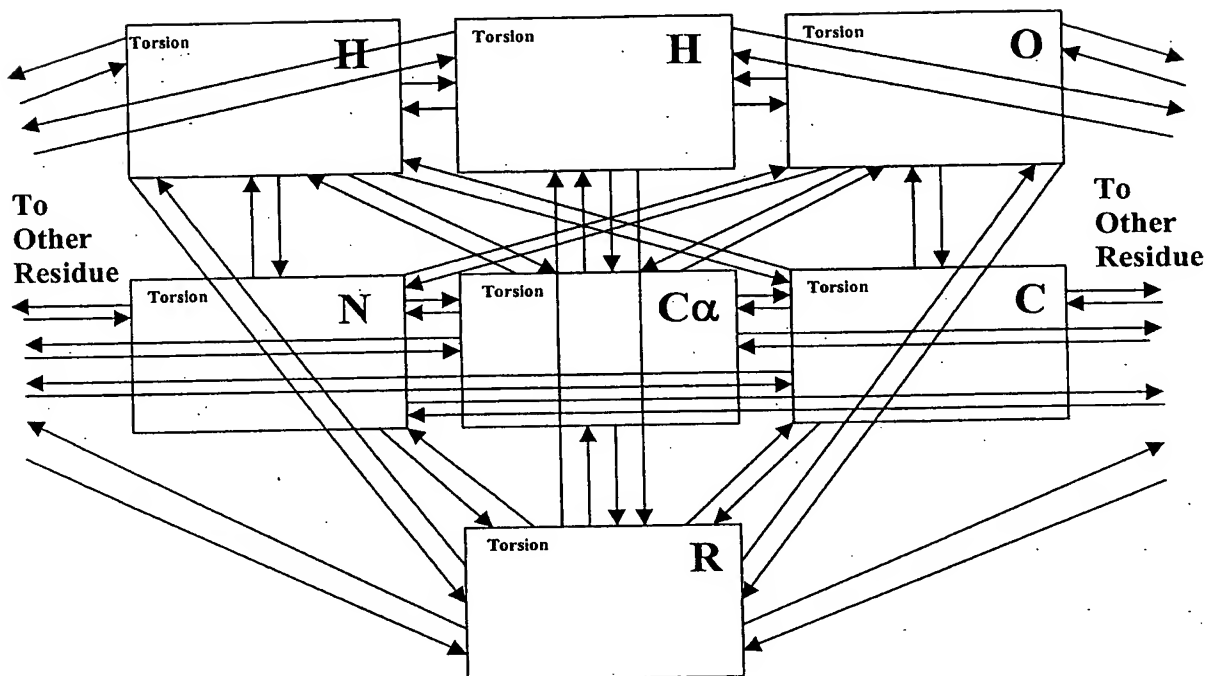


Figure 15

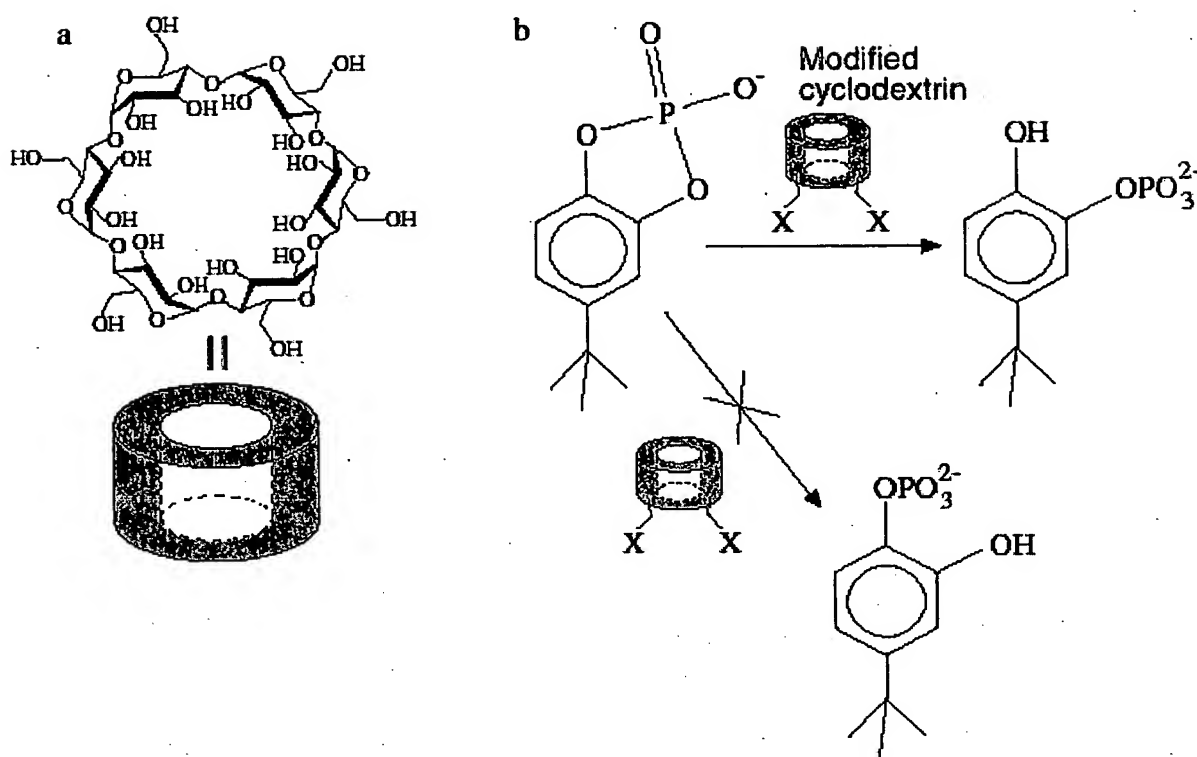


Figure 16

**Illustration of the Circuit Group
For a Sub-Unit in Cyclodextrin
(Bond Stretch Connections)**

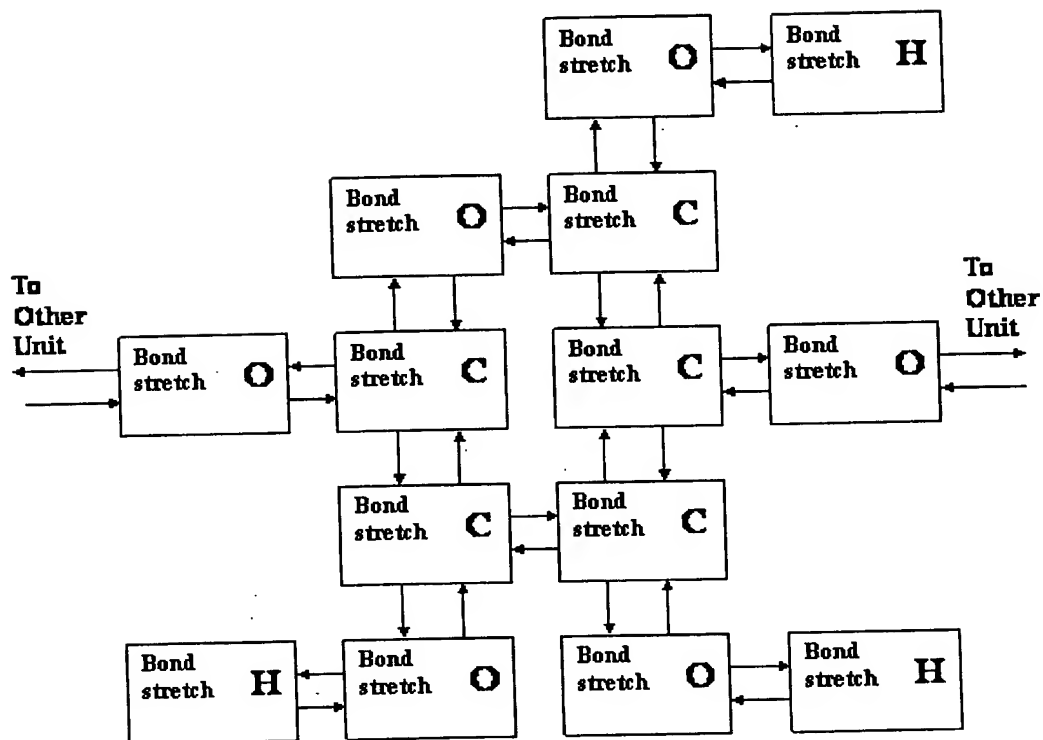


Figure 17

Figure 18

**Illustration of the Circuit Group
For a Sub-Unit in Cyclodextrin
(Angle Bending Connections)**

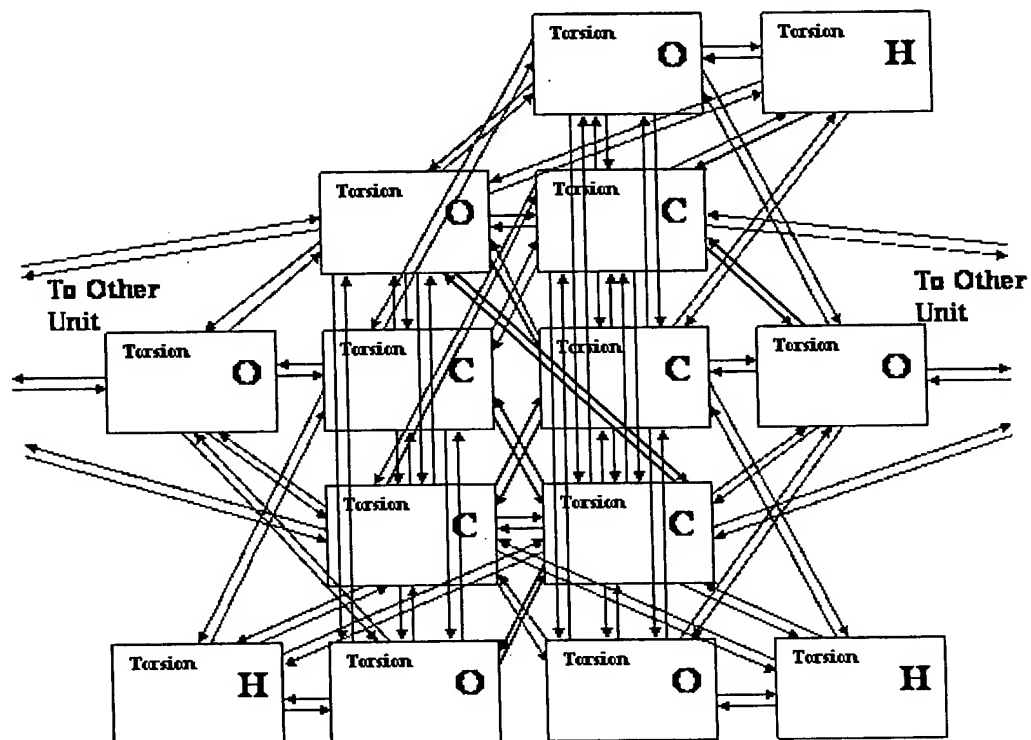


Figure 19

Bond Stretch X Unit

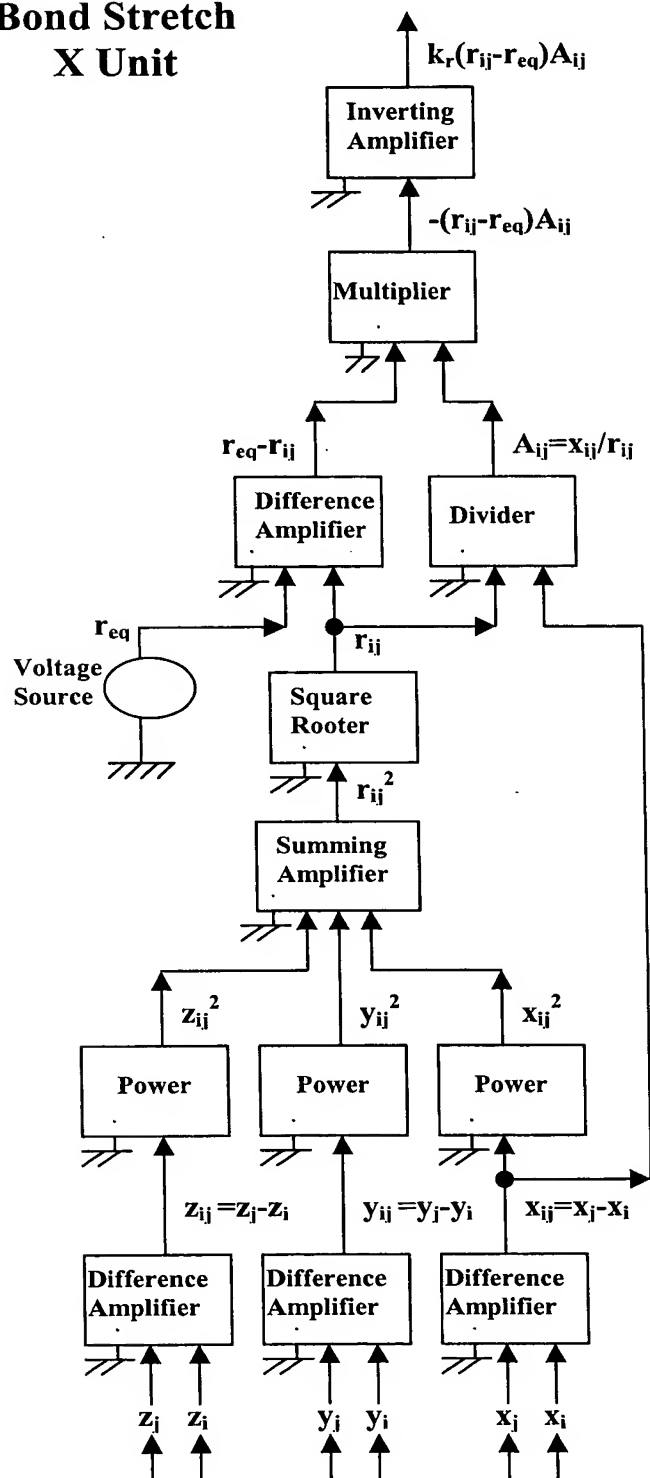


Figure 20

Bond Stretch Y Unit

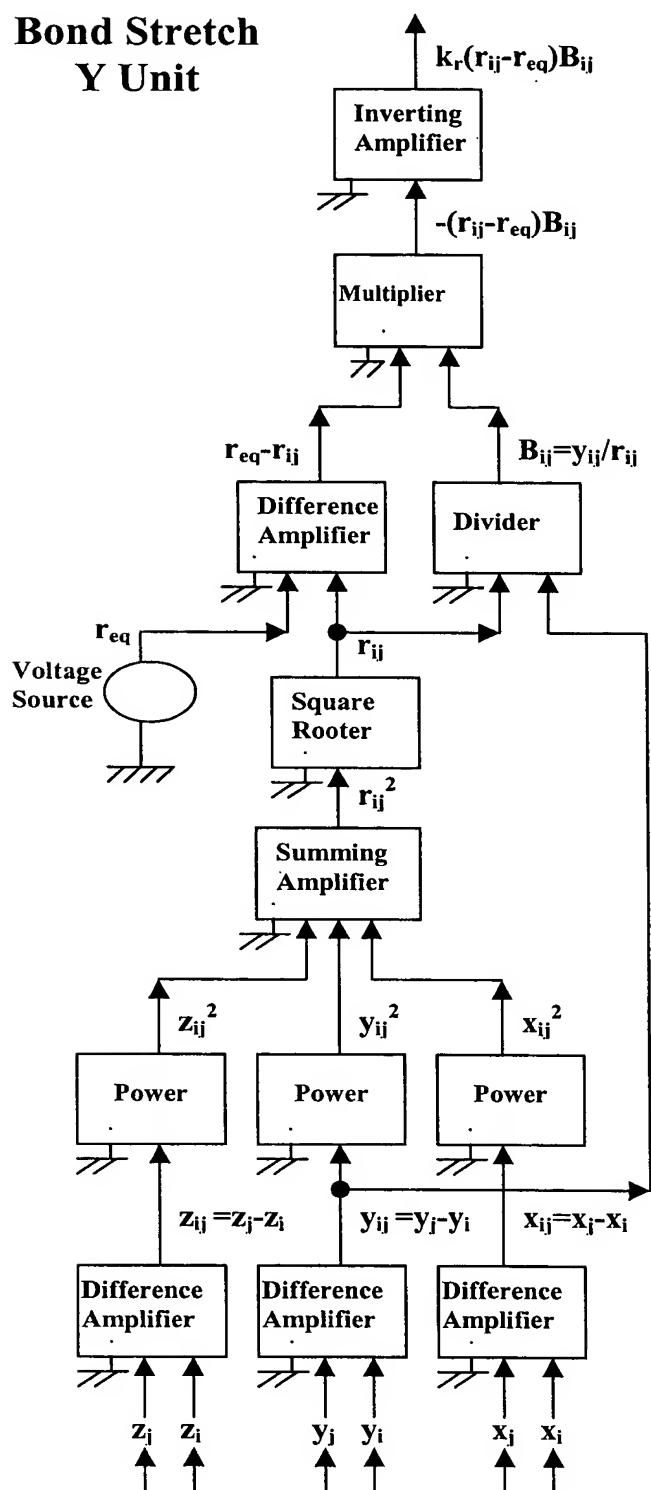


Figure 21

Bond Stretch Z Unit

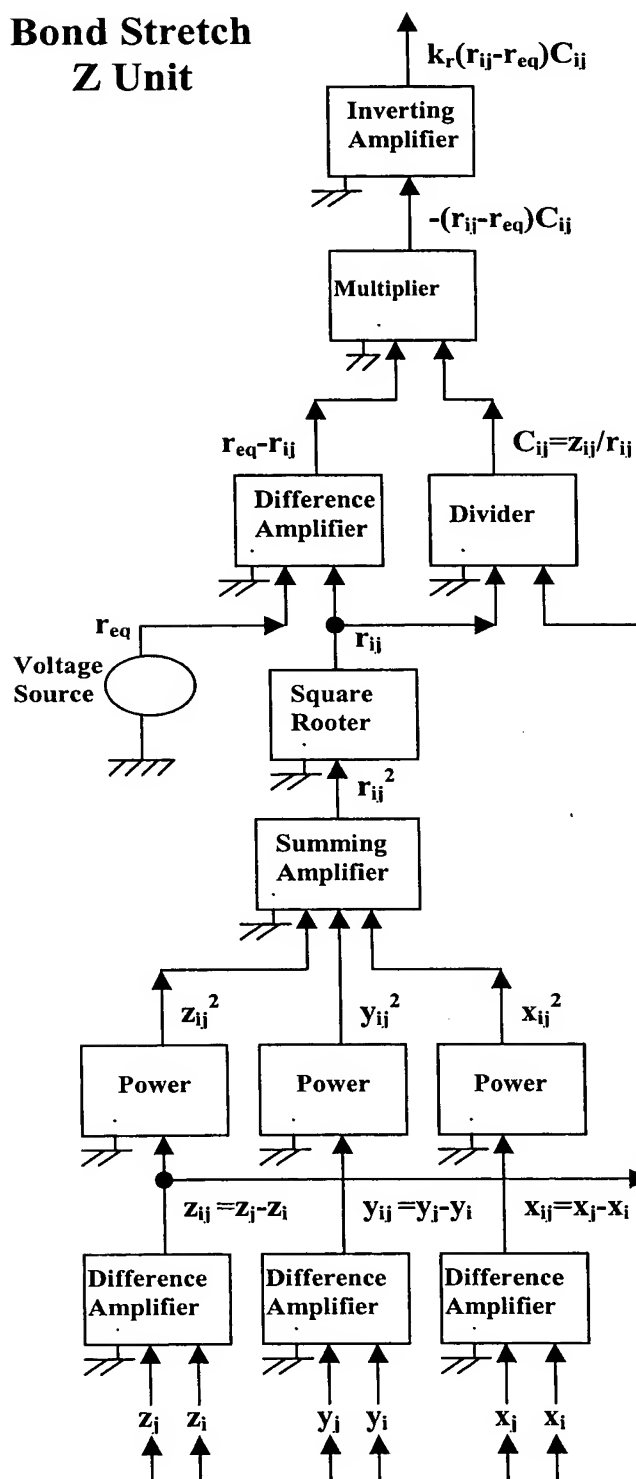


Figure 22

Angle Bending
X Unit
Type A

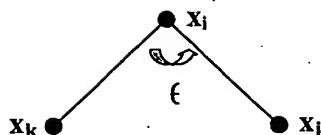
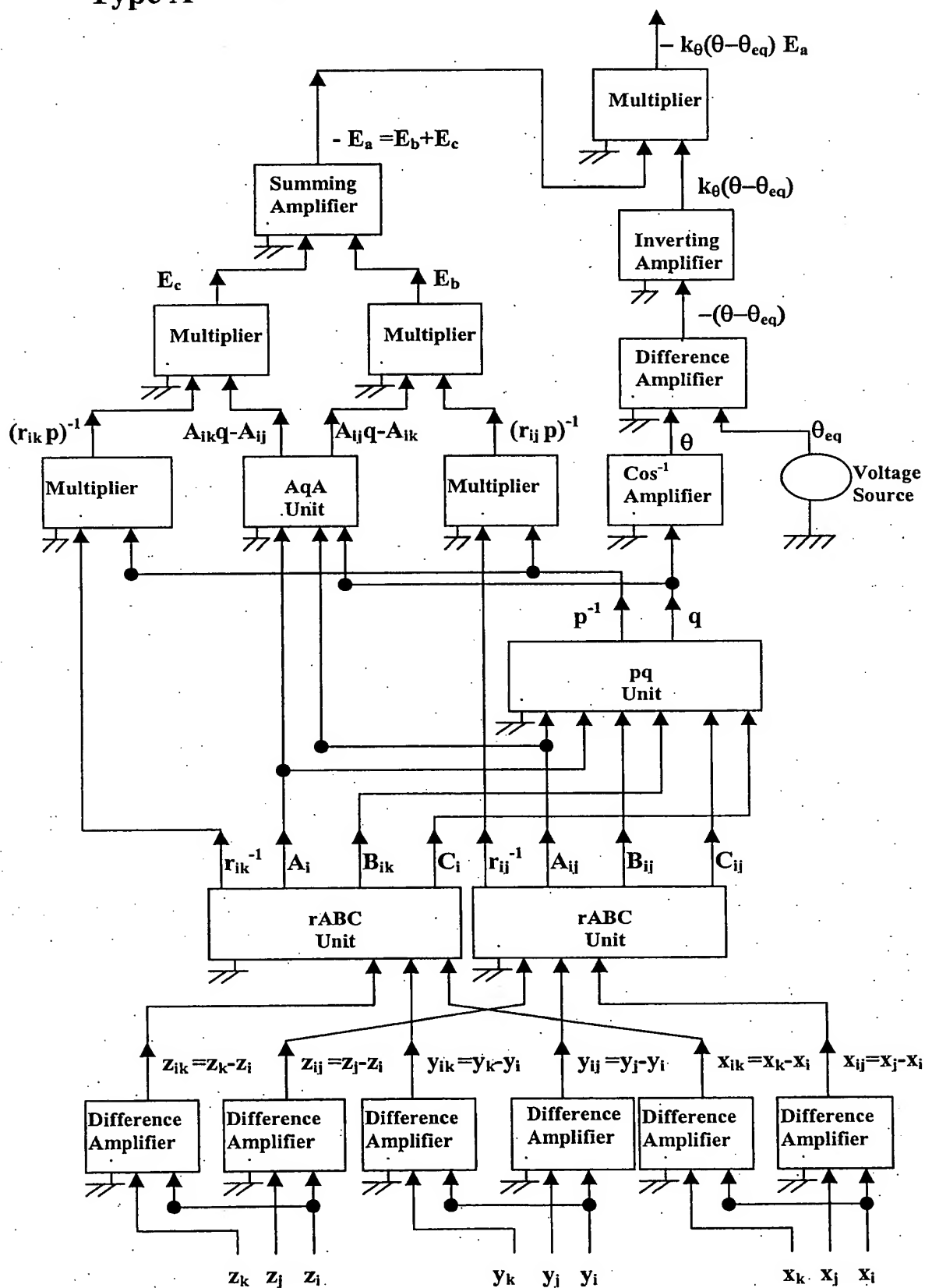


Figure 23



Angle Bending
X Unit
Type B

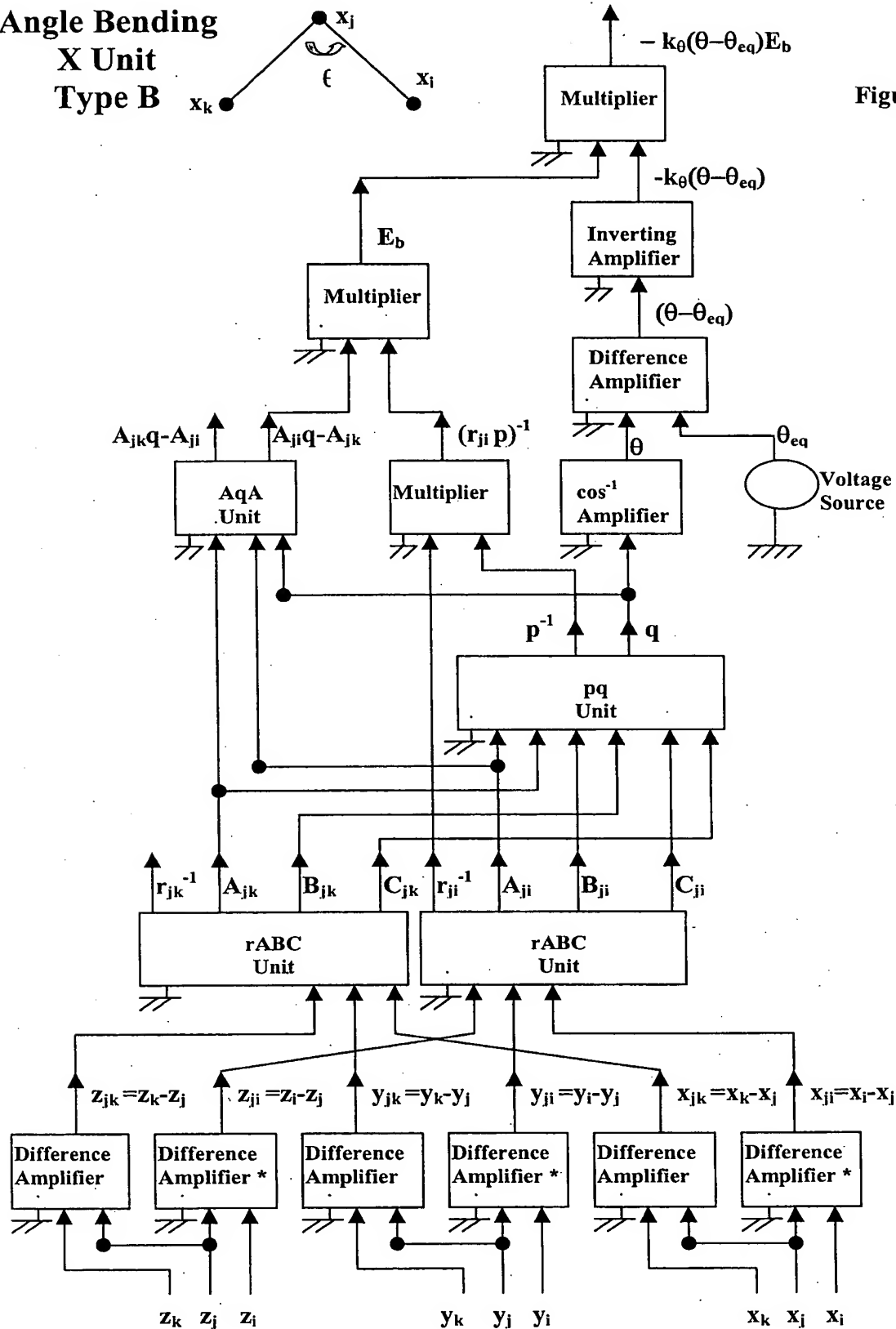


Figure 24

Angle Bending
Y Unit
Type A

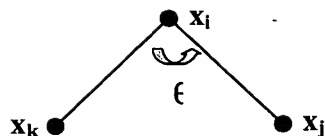


Figure 25

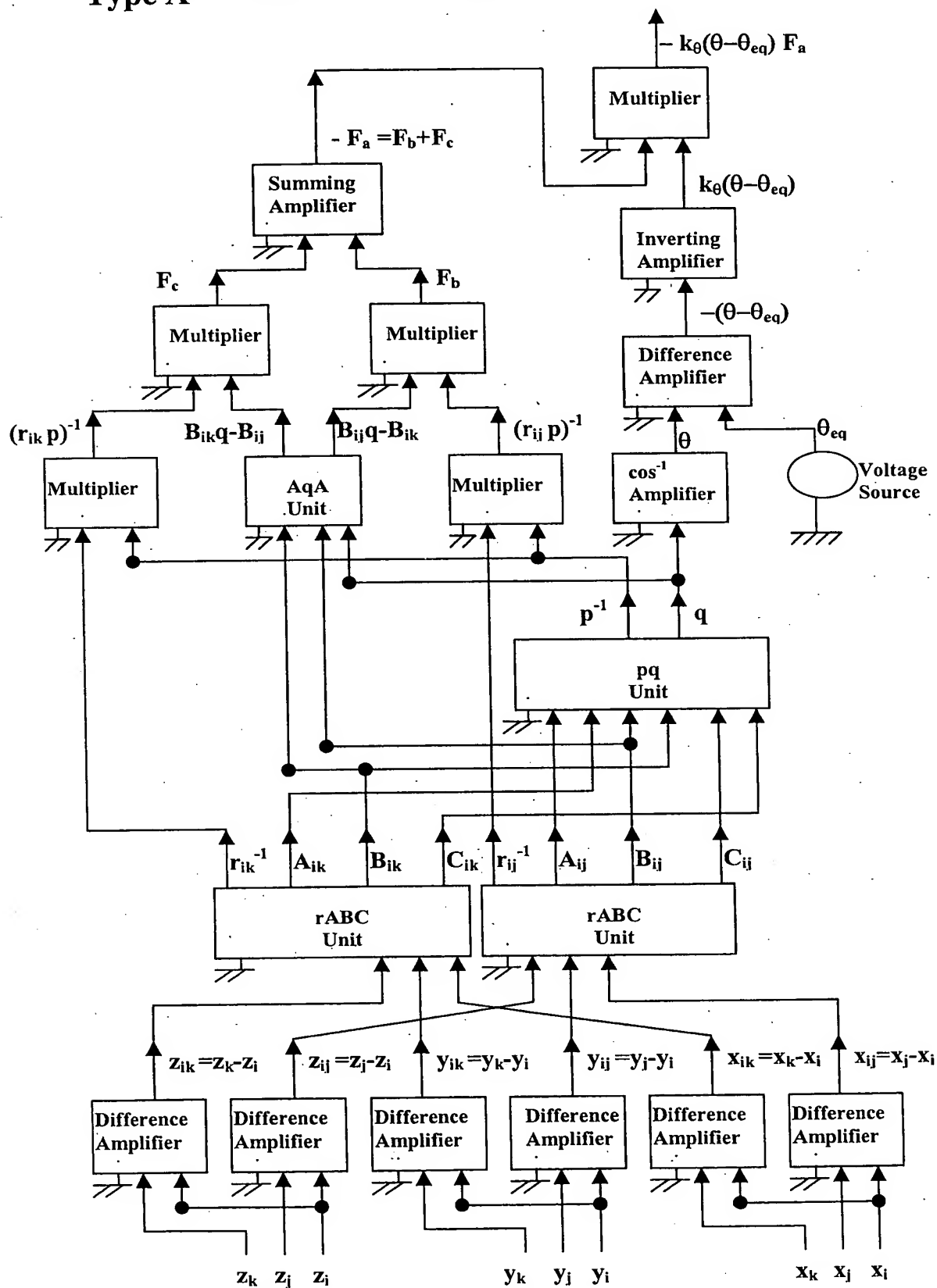
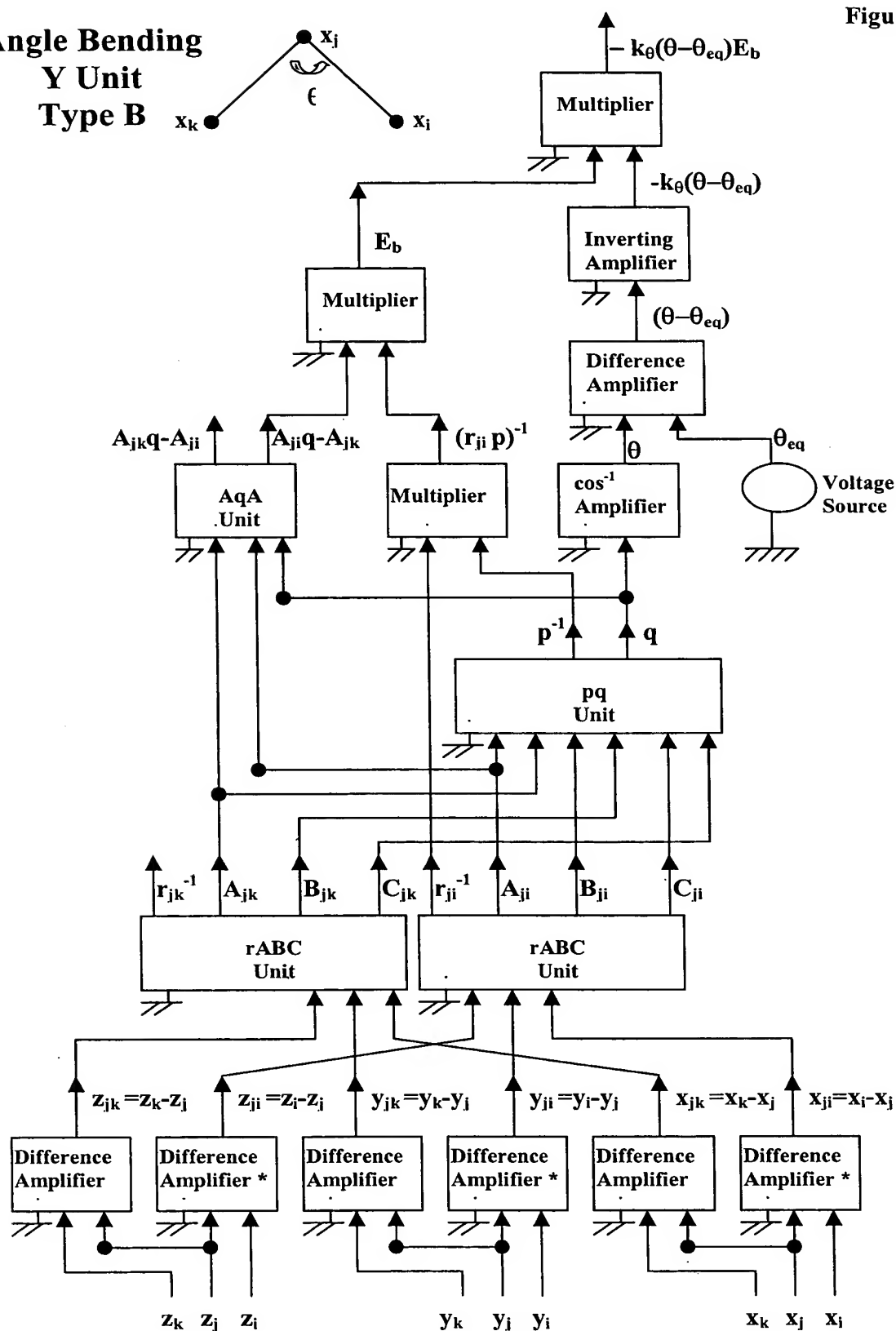


Figure 26

Angle Bending
Y Unit
Type B



Angle Bending
Z Unit
Type A

Figure 27

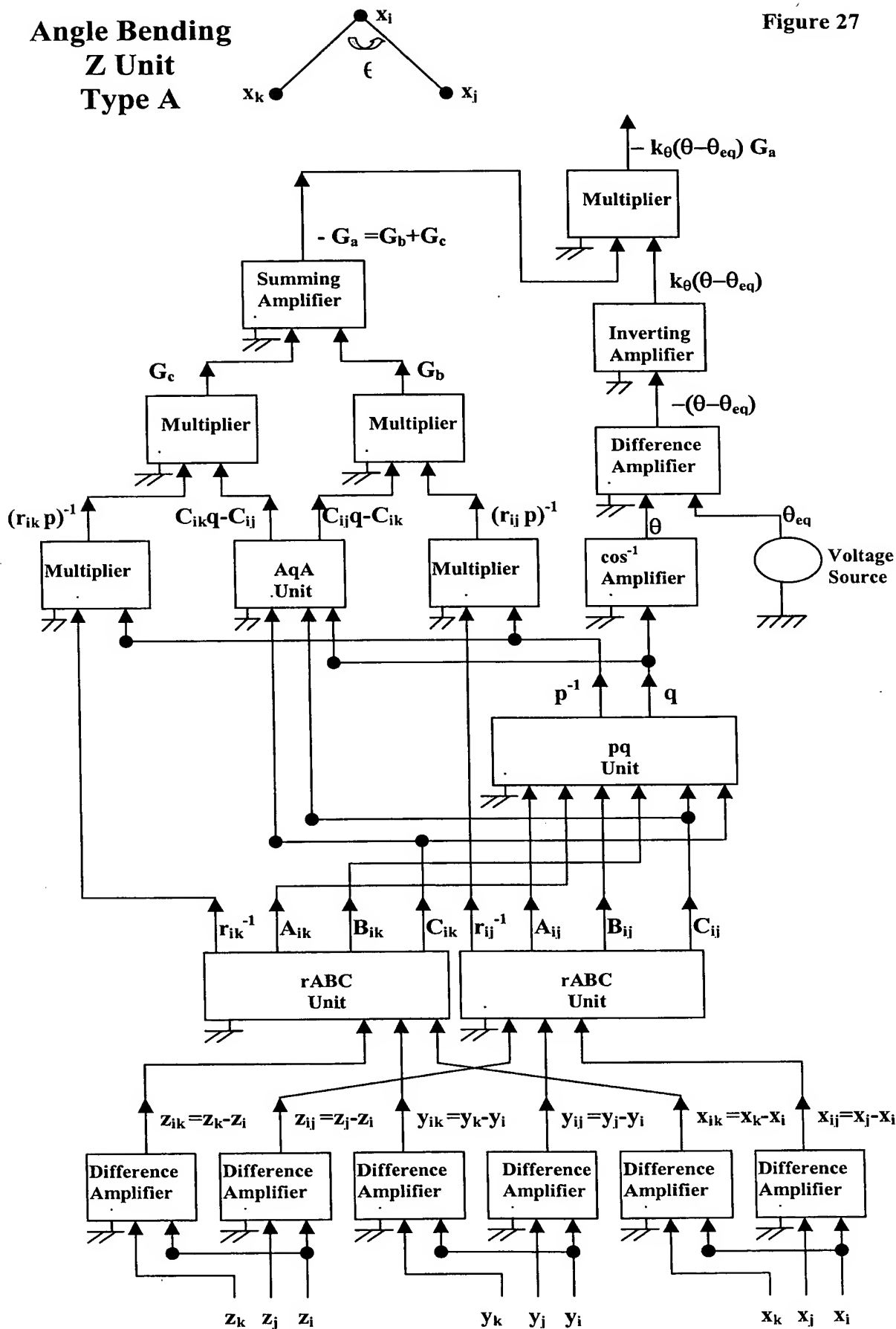
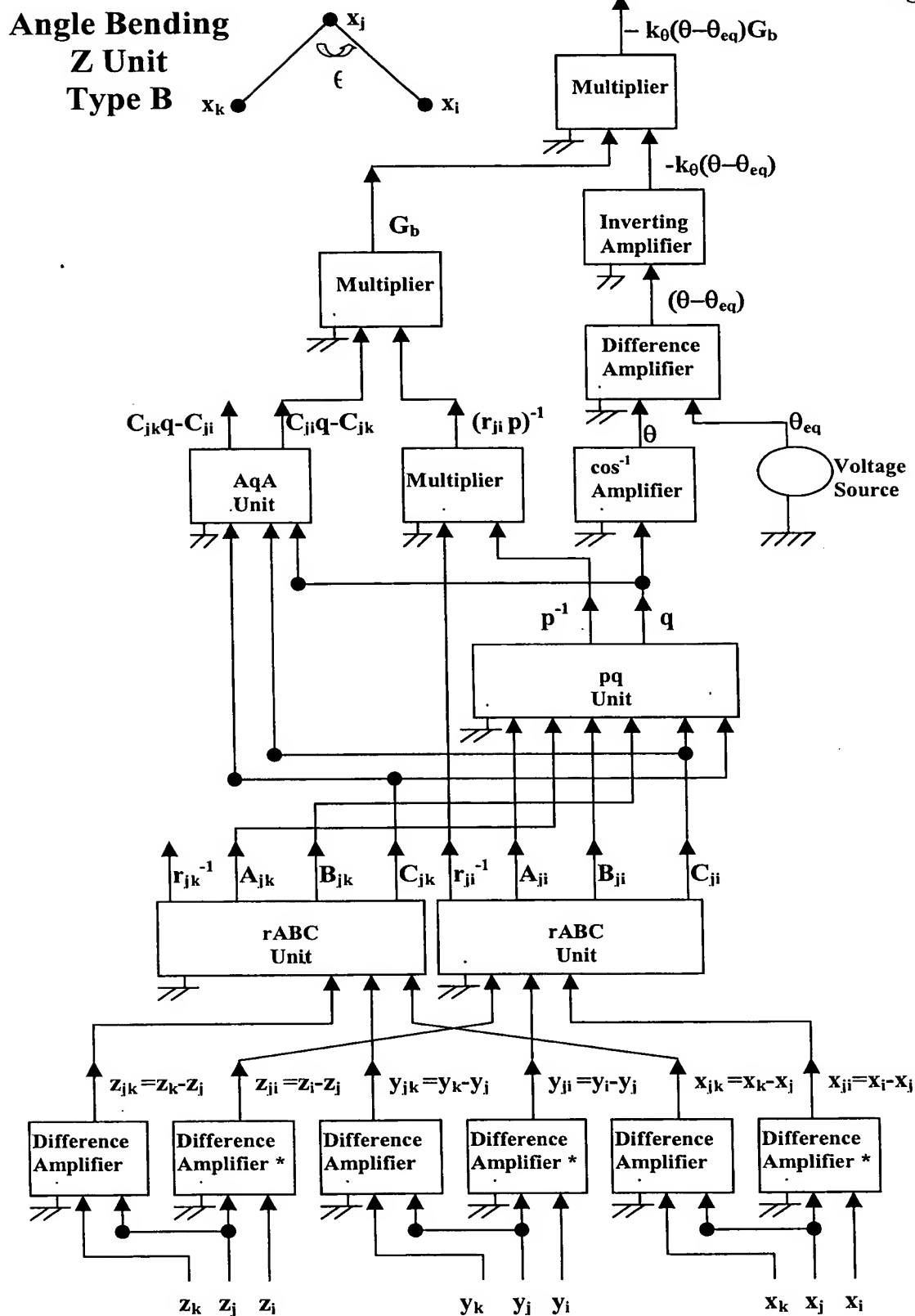
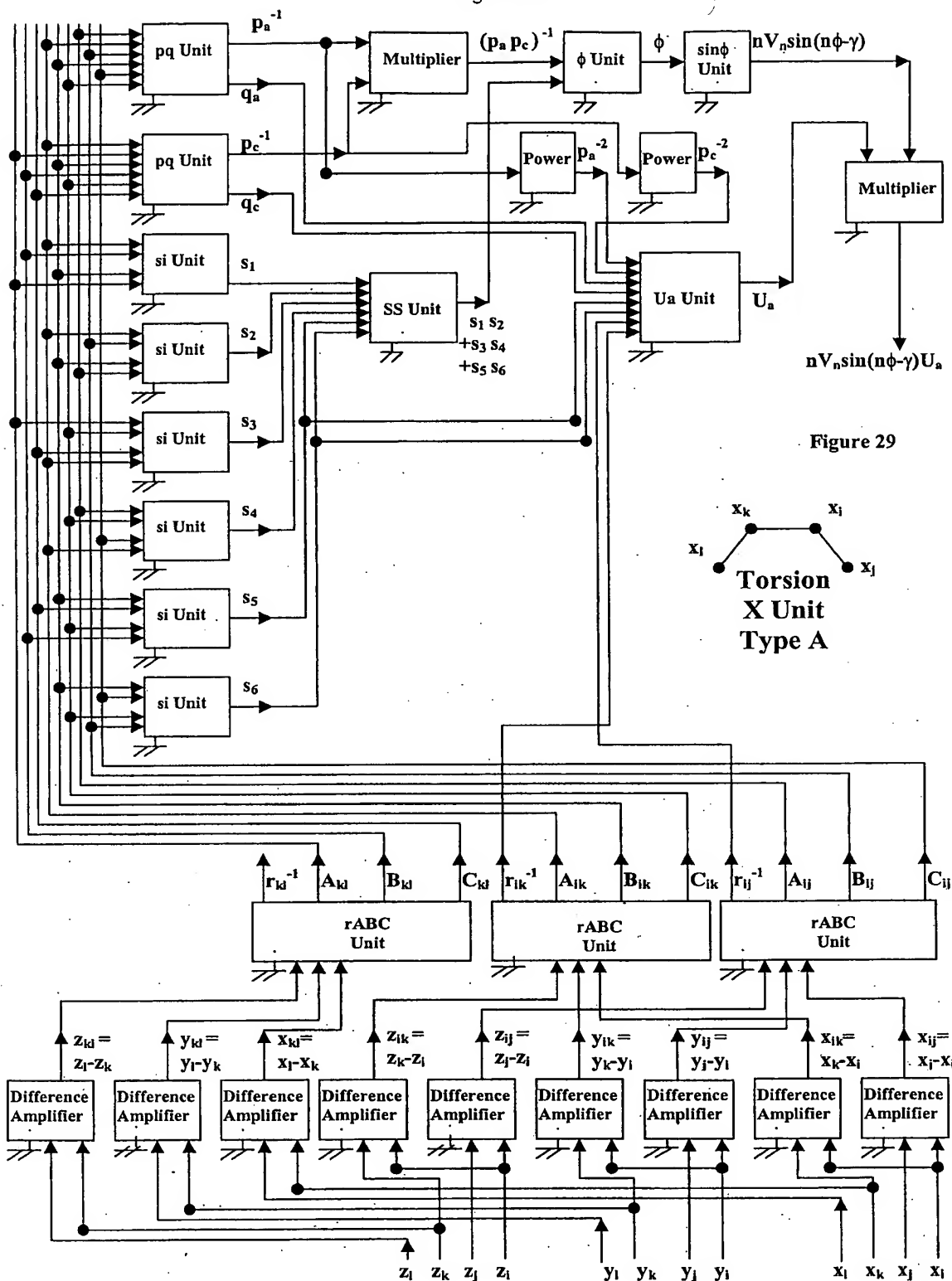


Figure 28





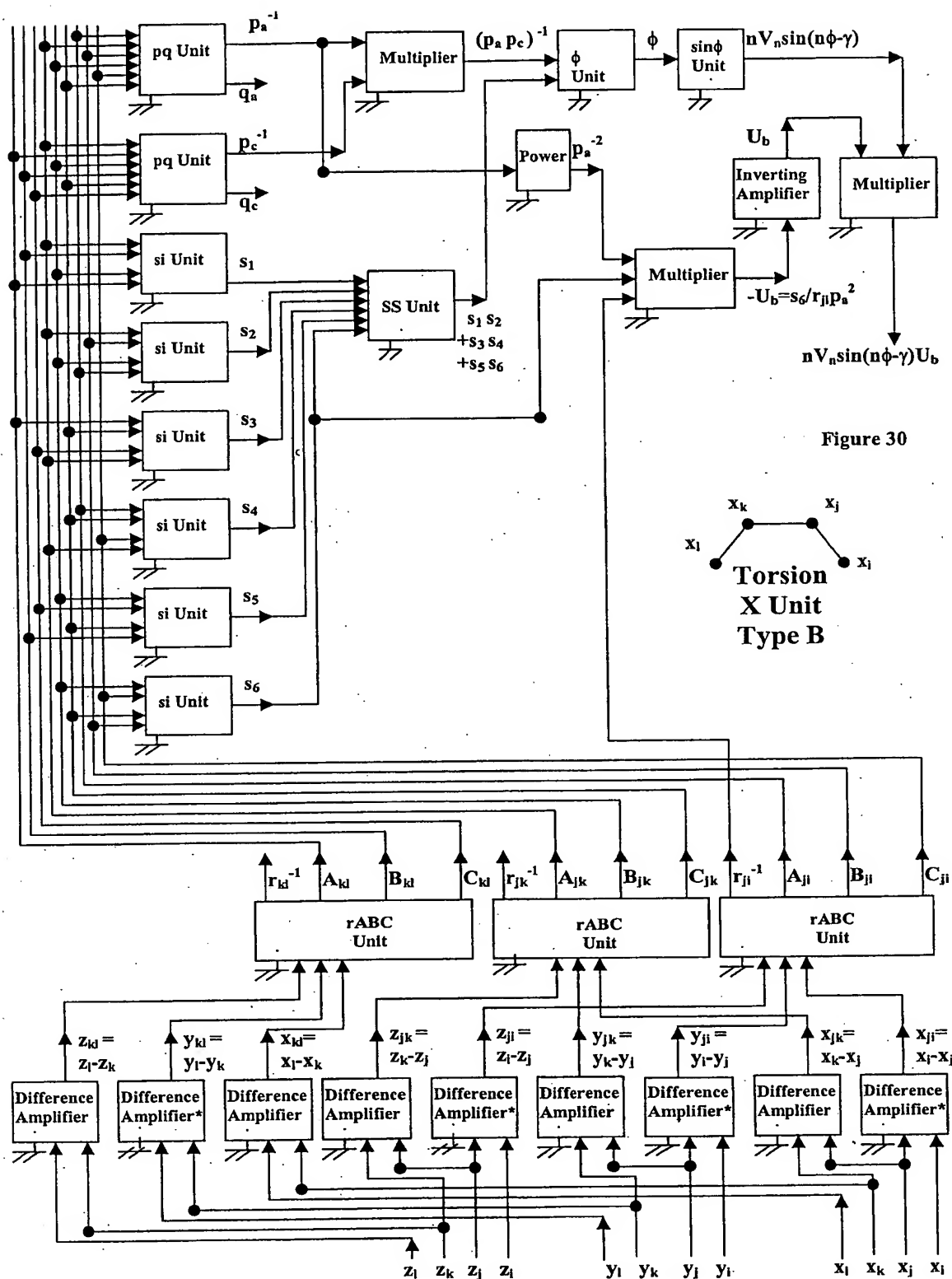


Figure 30

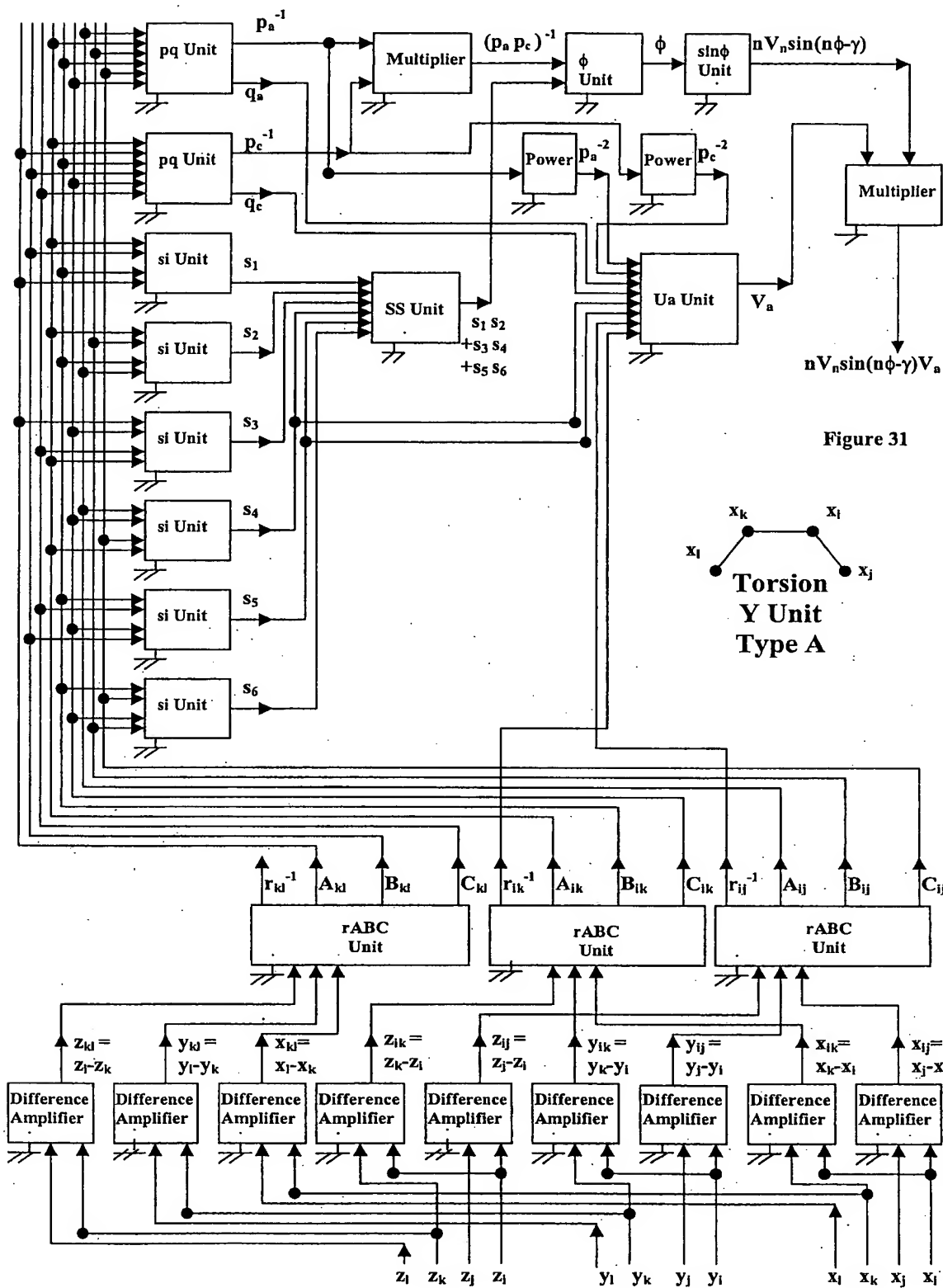


Figure 31

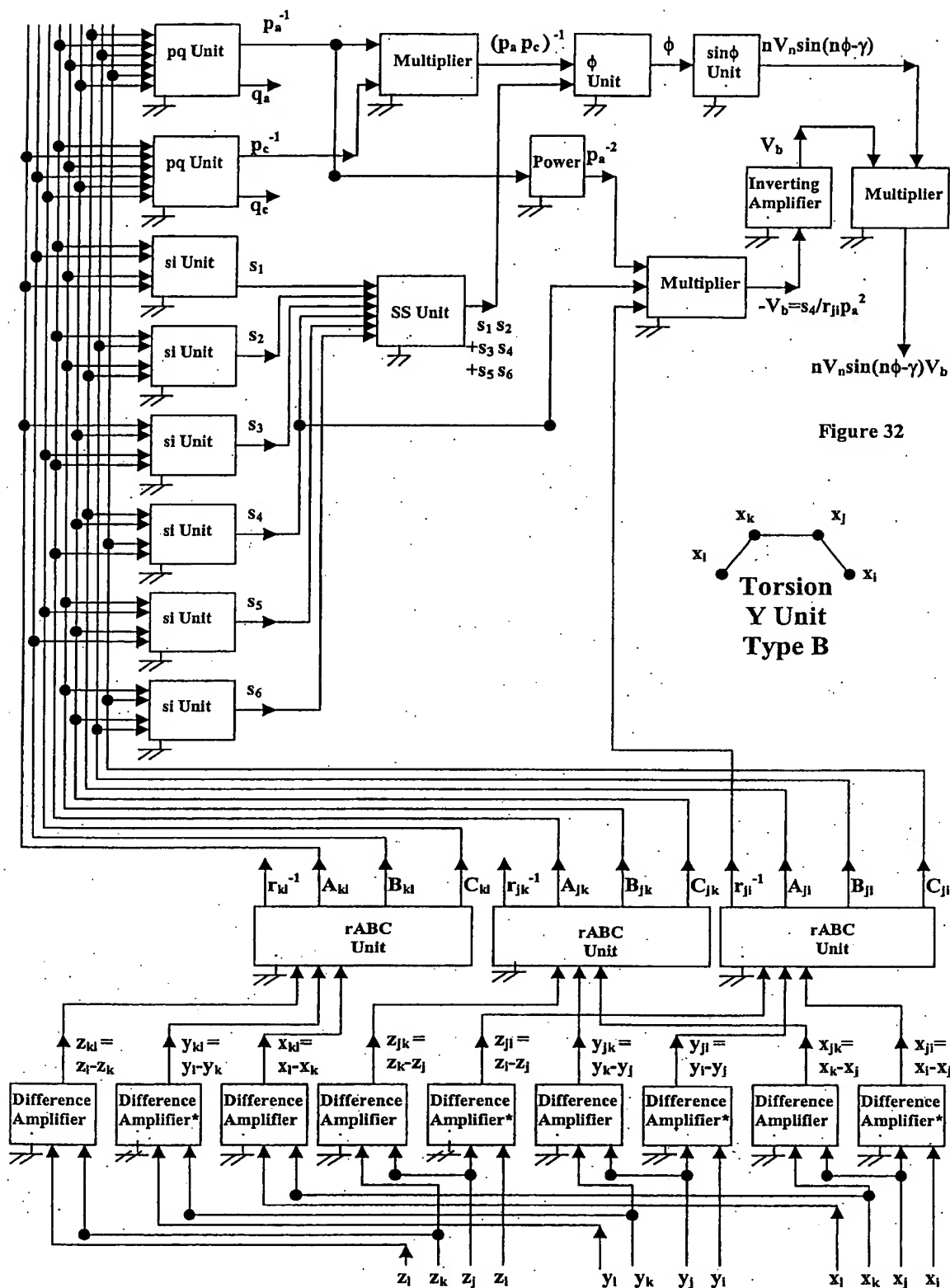


Figure 32

x_k x_j
 x_l x_1
Torsion
Y Unit
Type B

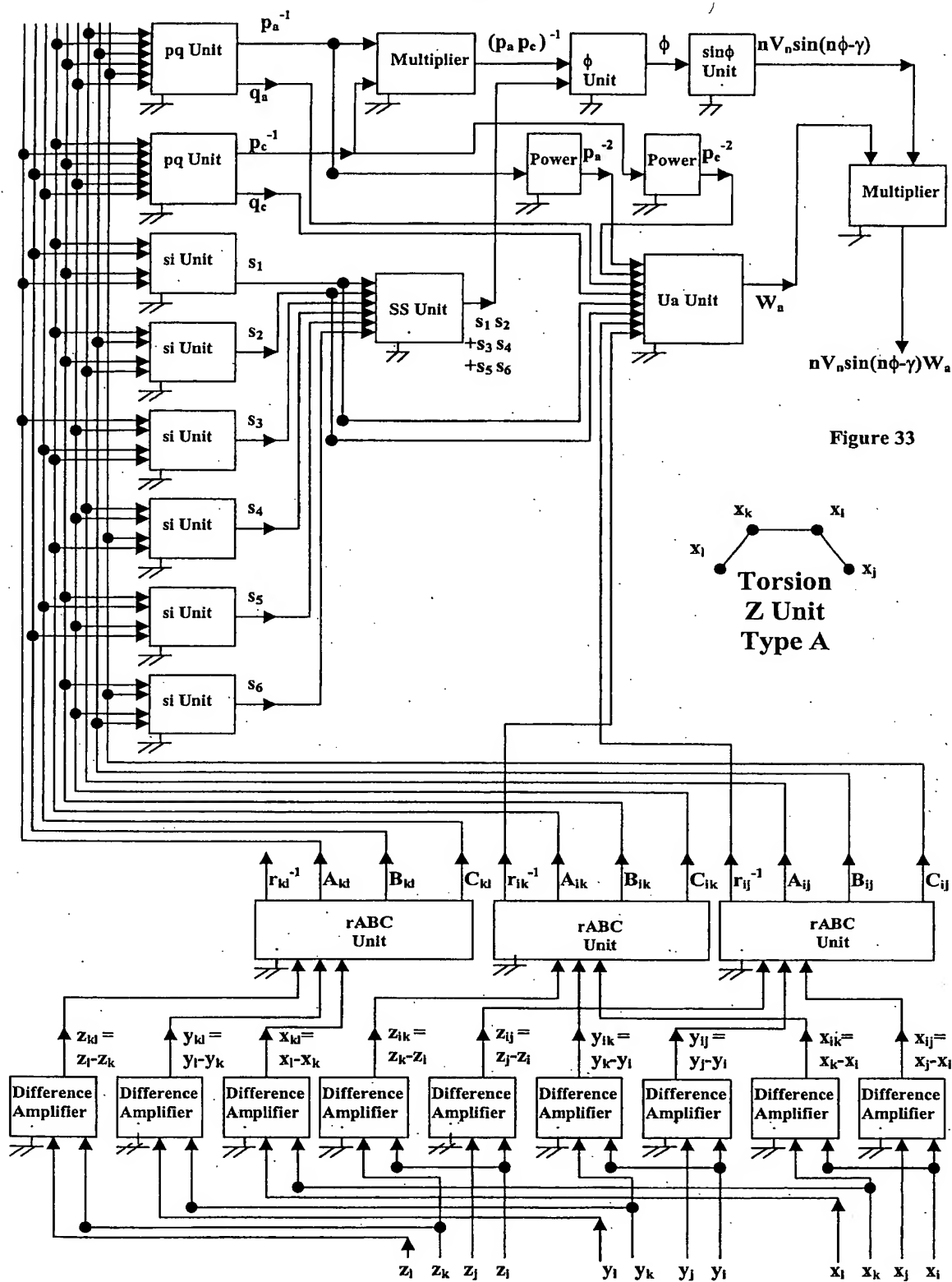


Figure 33

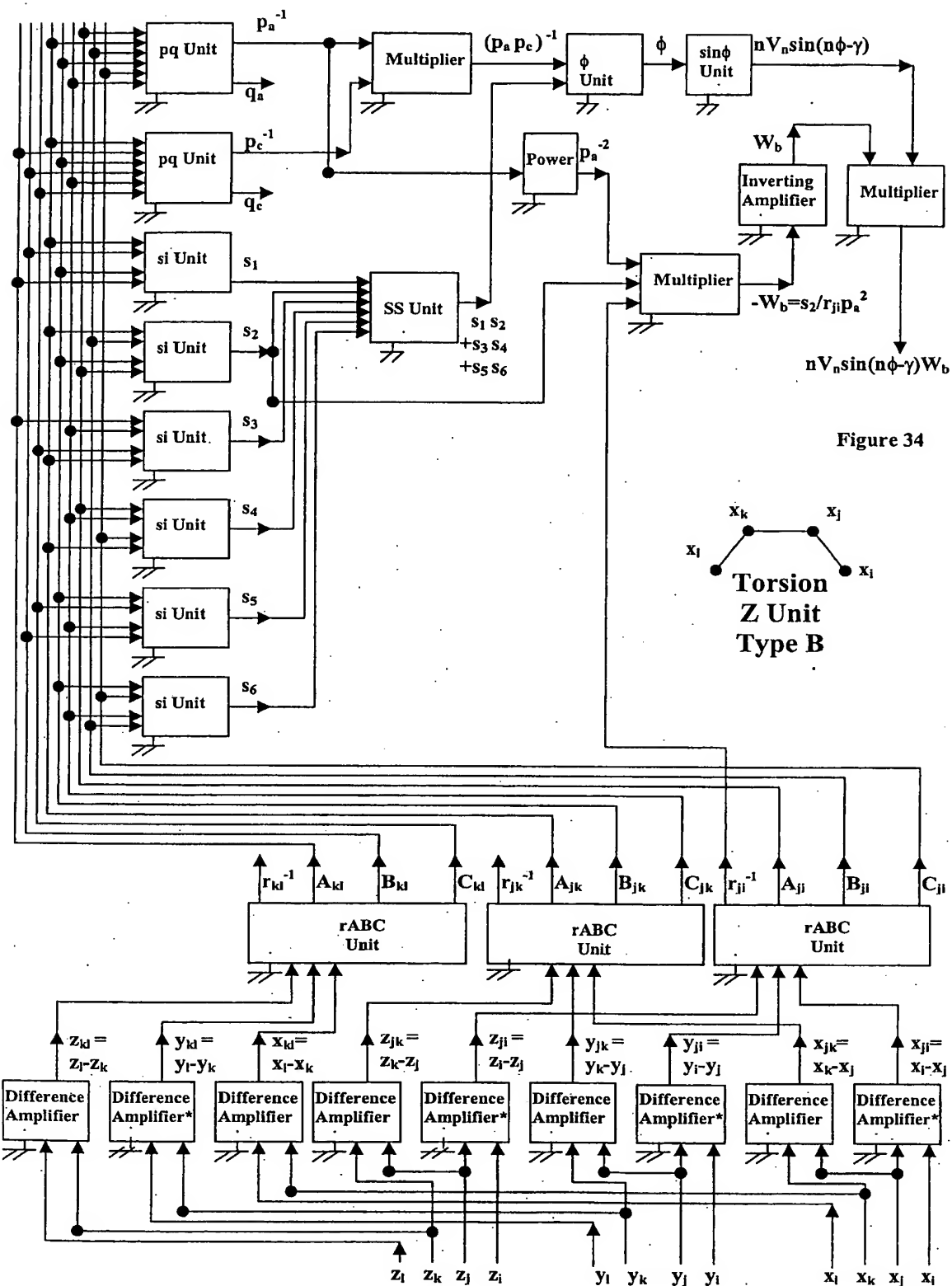
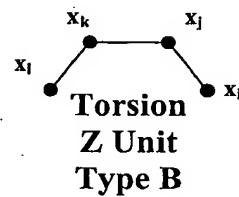


Figure 34



Non-bonded X Unit

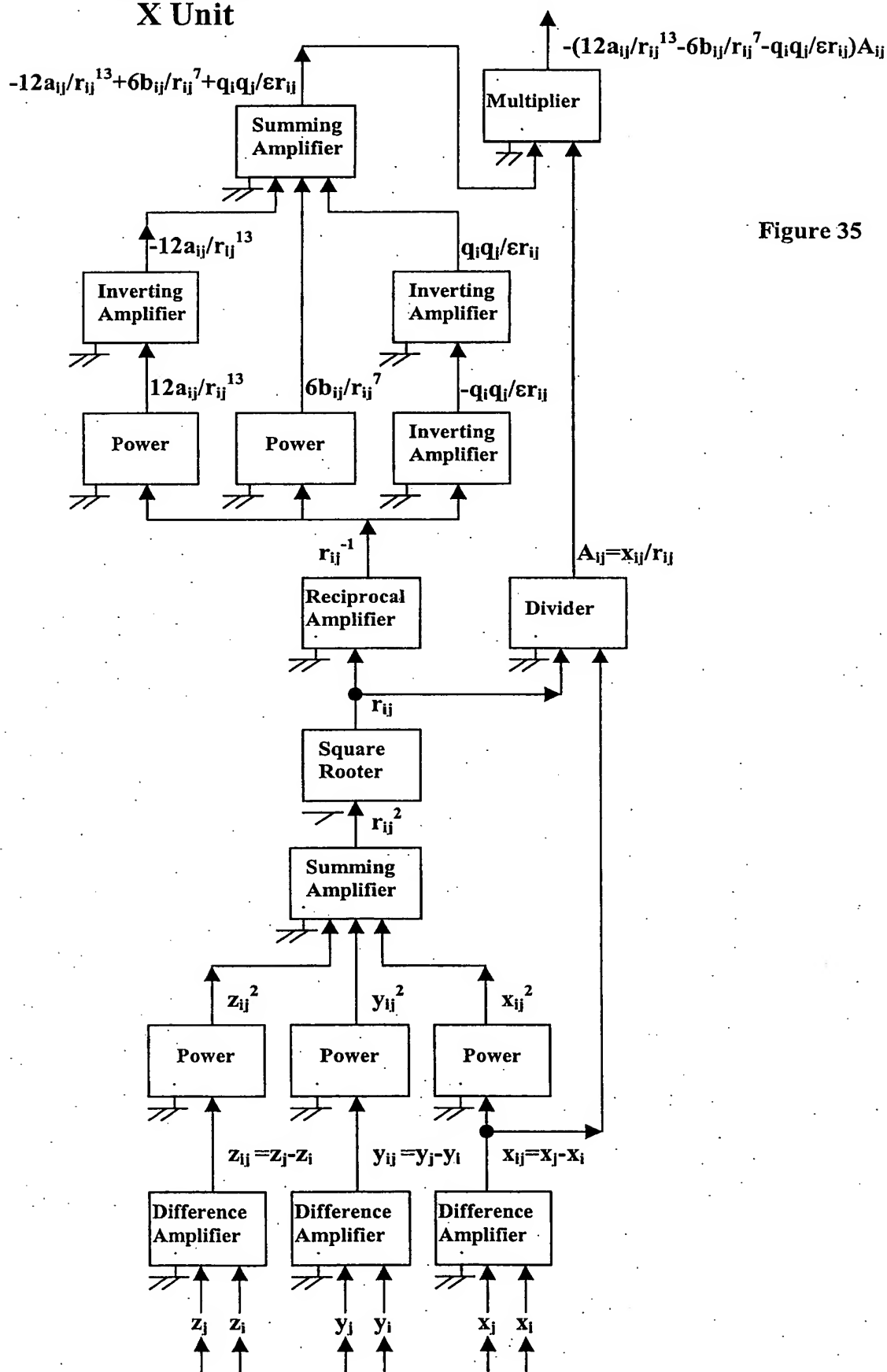


Figure 35

Non-bonded Y Unit

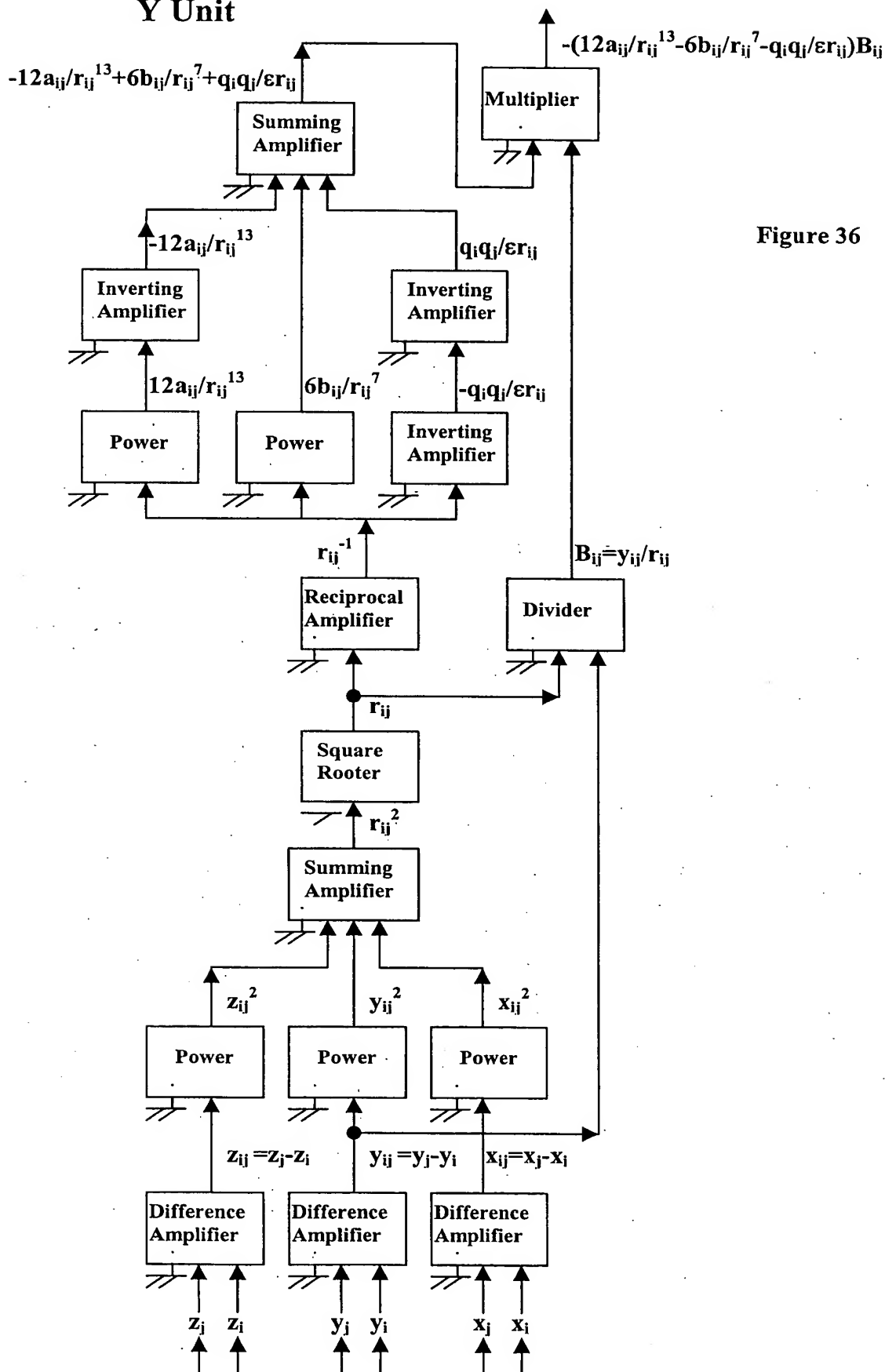


Figure 36

Non-bonded Z Unit

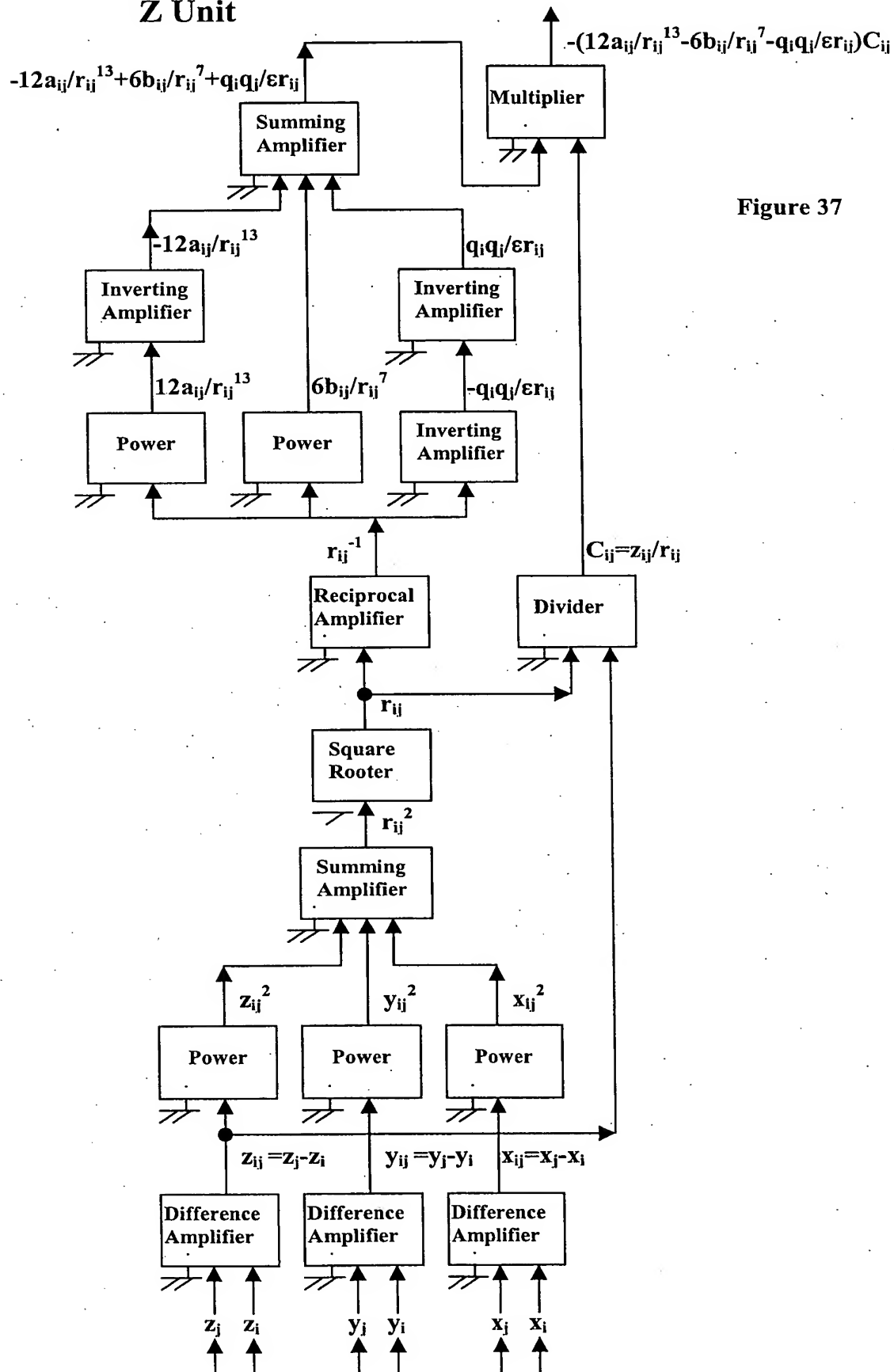


Figure 37

H-bond
X Unit

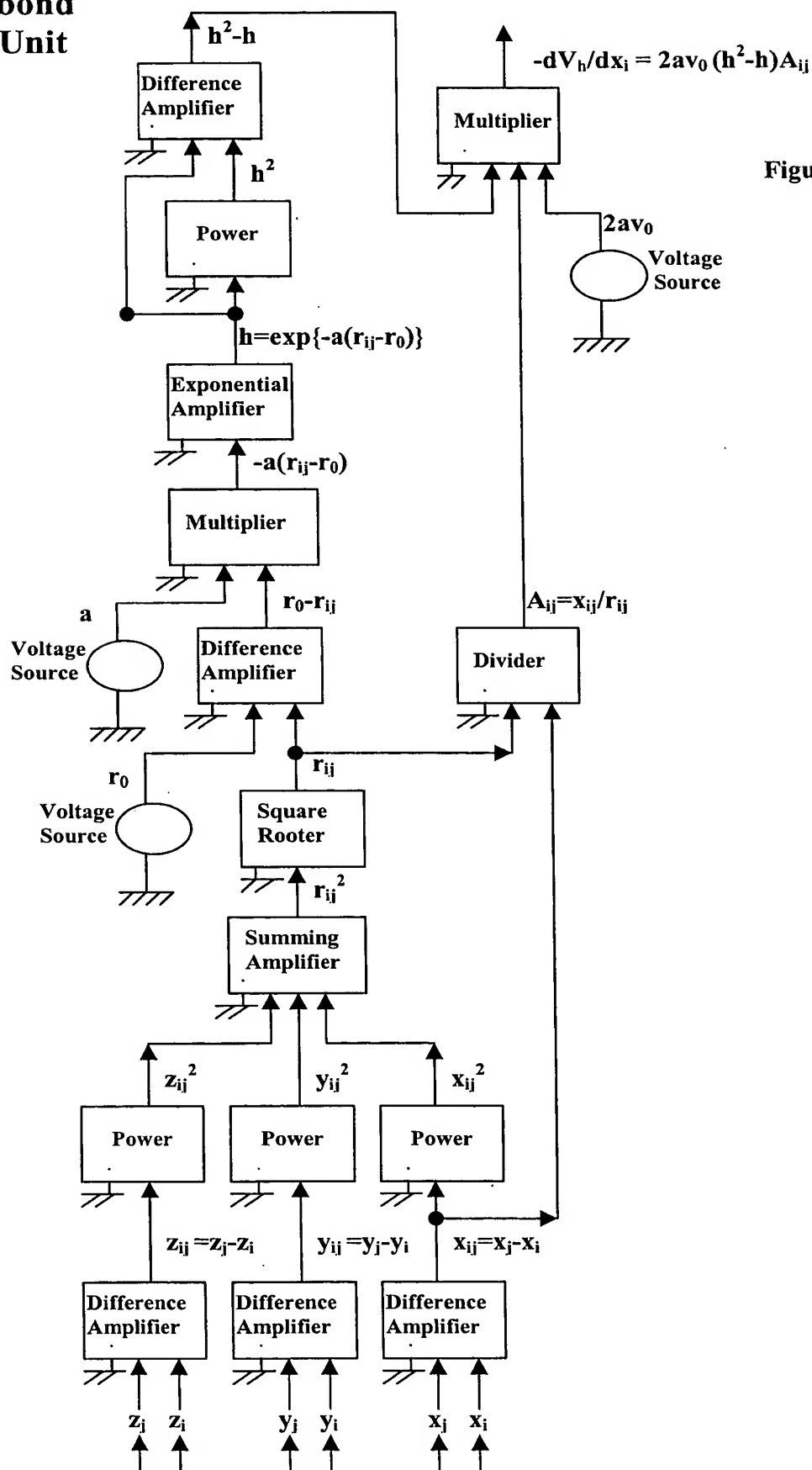


Figure 38

H-bond Y Unit

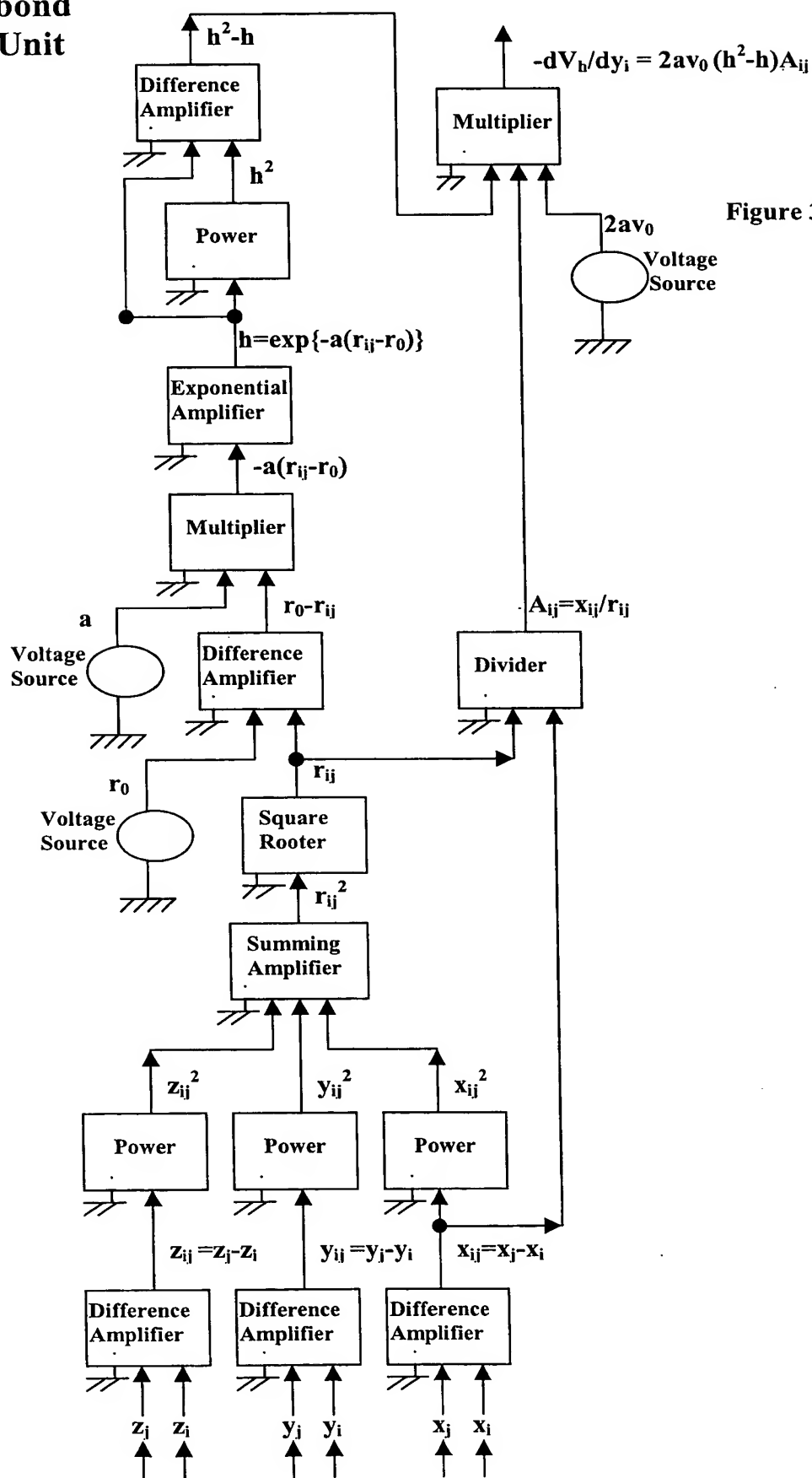


Figure 39

H-bond Z Unit

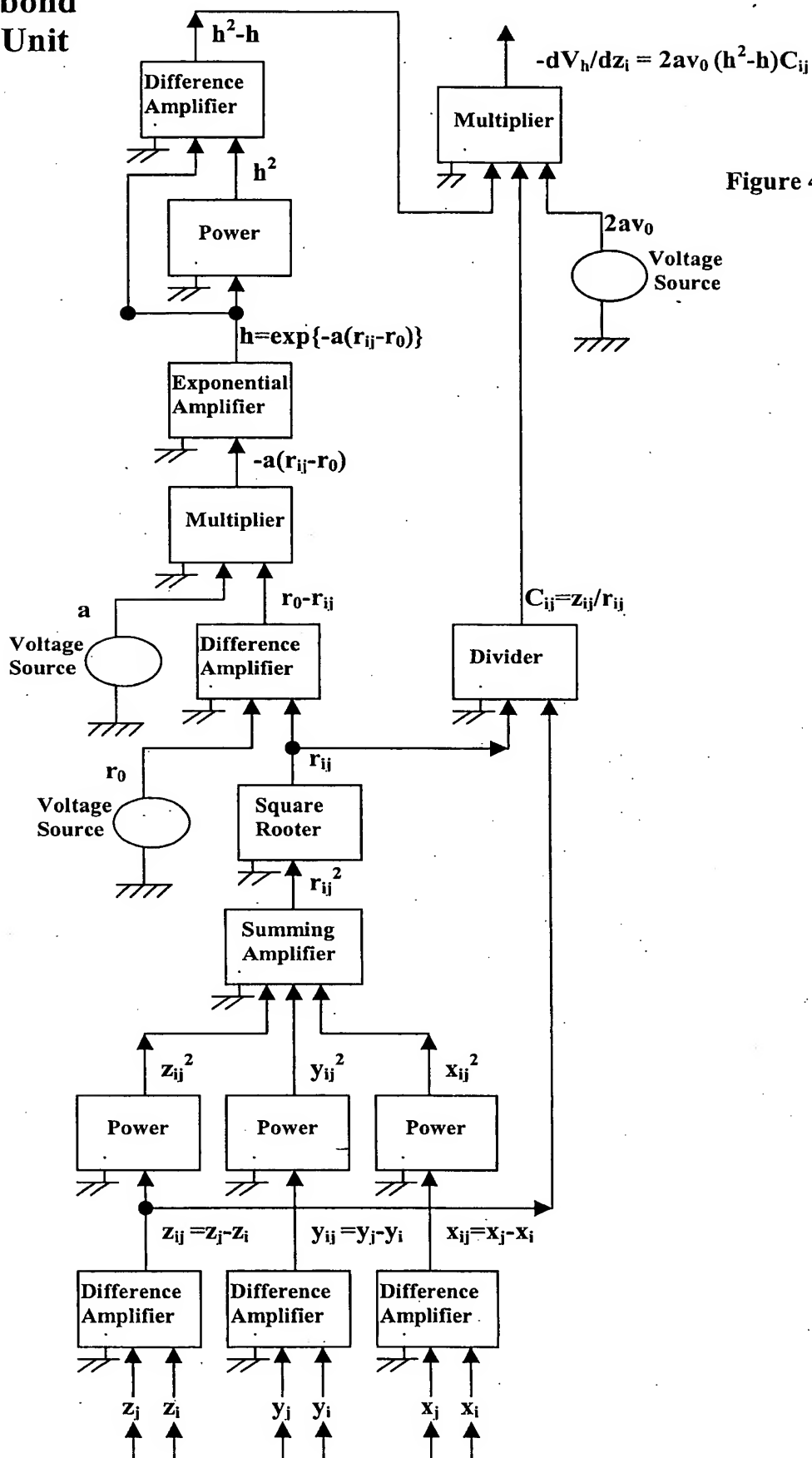


Figure 40

rABC Unit

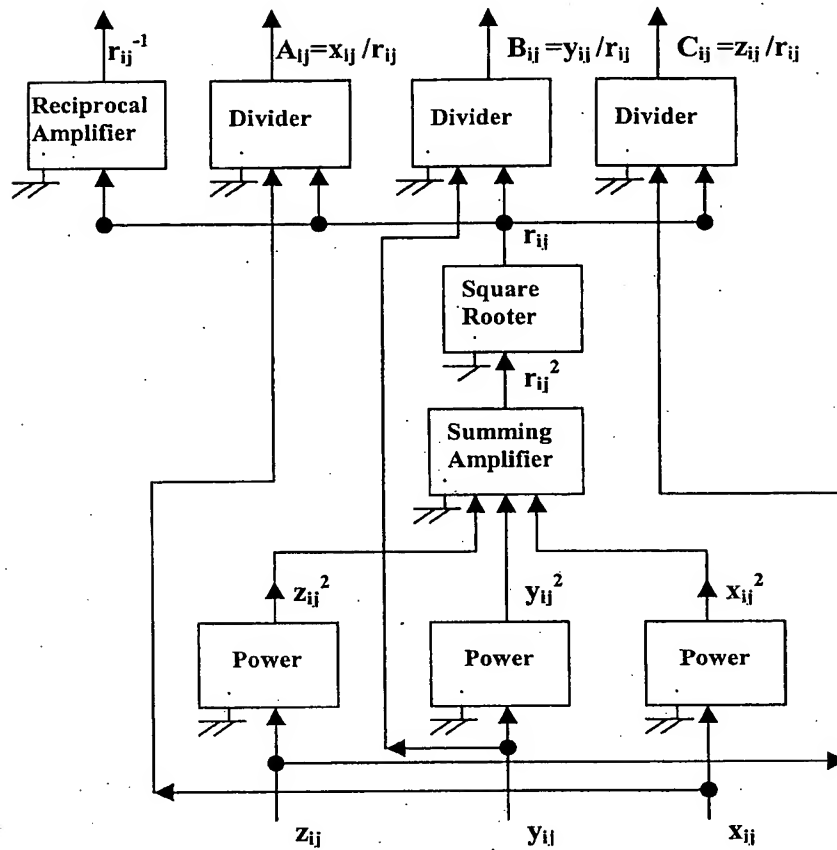
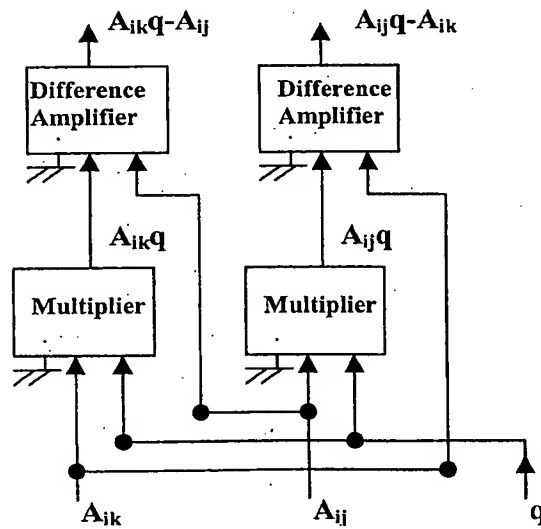
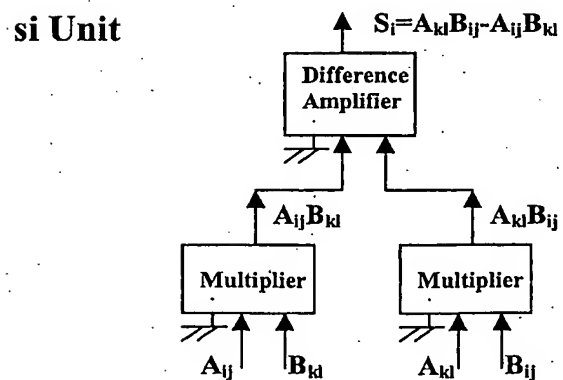


Figure 41

AqA Unit





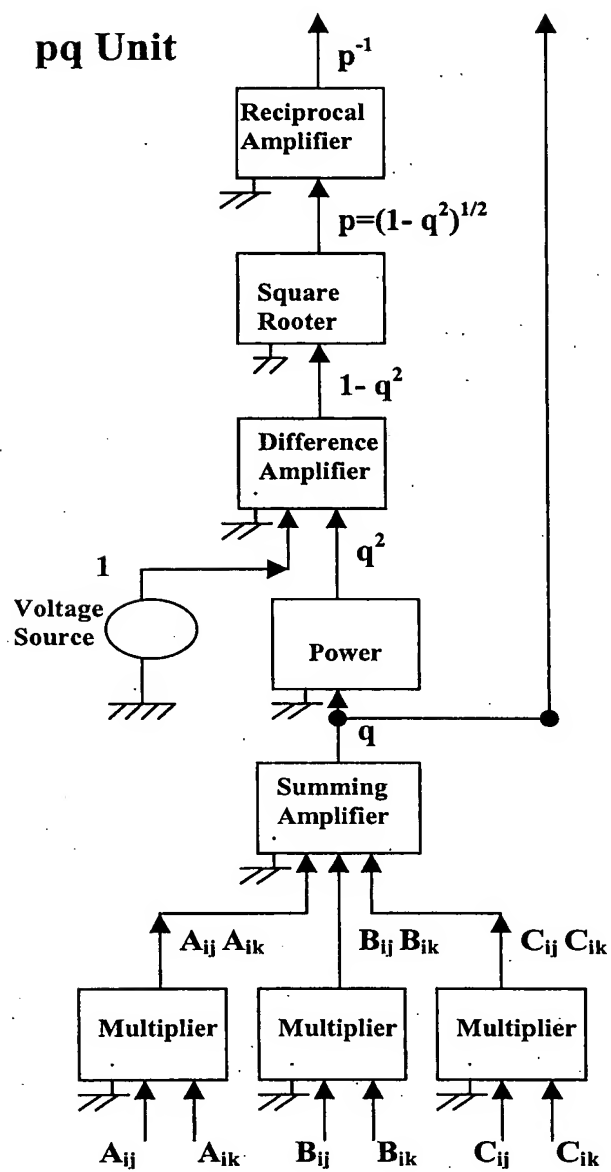


Figure 43

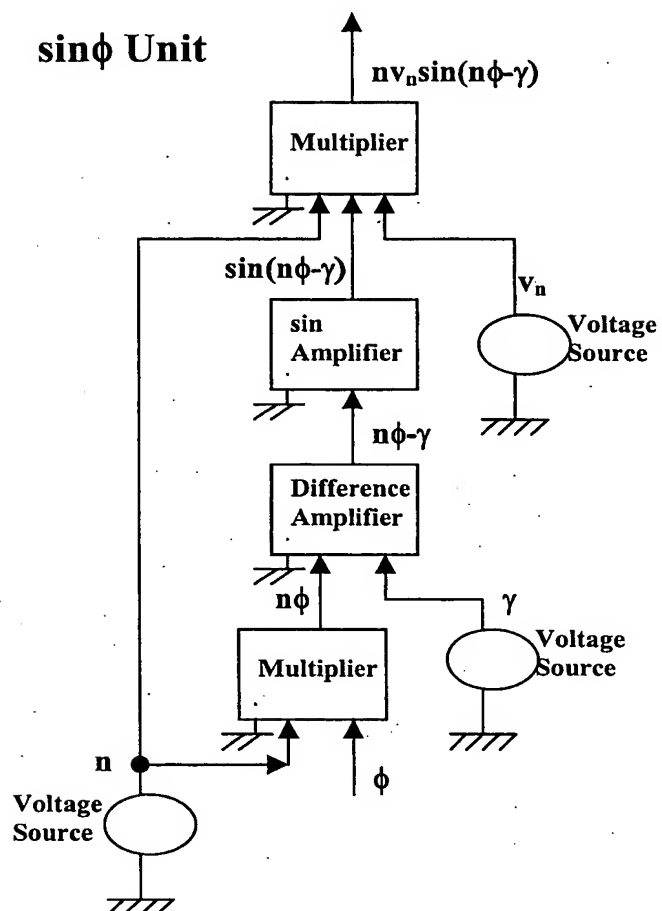


Figure 44

